Predicting the Strength of Metal-Support Interaction with Computational Descriptors for Adhesion Energies - Supplementary Information

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S1 Further Analysis and Details of the Calculations

S1.1 Formation of oxidized surfaces from hydroxylated surface

As mentioned in the main text, hydroxylated surface are thermodynamically most stable under most relevant conditions for α-SiO_2(0001), α-Al_2O_3(0001) and γ-Al_2O_3(110). The corresponding oxidizing surfaces are obtained by removing the hydrogen atoms (H) of the hydroxyl groups (OH). These oxidized surfaces only serve as an artificial reference to be able to directly compare the adhesion energies of oxidized surface to that of stoichiometric surfaces, which is otherwise difficult since the formation of oxidized interface from hydroxylated surfaces always depends on the chemical potential of hydrogen.

The shift $\Delta\gamma_{\mathrm{ox-lat}}^{\mathrm{ox}}$ that allows to relate all discussed adhesion energies referenced to the oxidized surface ($\gamma_{\mathrm{adh}}^{\mathrm{ox}}$) to hydroxylated surfaces ($\gamma_{\mathrm{adh}}^{\mathrm{hydrox}}$) is listed in Table S1. The clean oxidized oxide surfaces derived from the hydroxylated surfaces by removing the surface hydrogen atoms (H) were optimized only for the unstrained oxide, using spin-polarized calculations. We note that the obtained structures are not very stable and partially react under the formation of peroxo structures, e.g. under the formation of O-O bonds. However, the energetic difference between different oxidized structures using different supercells and magnetic states turned out to be relatively small (30 meV/Å^2) compared to $\Delta\gamma_{ox-lat}^{ox}$. No zero-point vibrational correction is applied. Adhesion free energies for any temperature and H_2-pressure can be obtained by computing the free energy of H_2 at those conditions, multiplying by the number of formed hydrogen atoms per unit cell (n/2, see Table S1) and dividing by the unit cell area (Table S8). In this way one can also easily compute the adhesion free energy in the presence of O_2, if H_2O is formed, by adding the reaction free energy for the formation of H_2O.

Table S1. Surface energy difference between hydroxylated and oxidized surface, if H_2 is liberated. $\Delta\gamma_{ox-lat}^{ox}$ is listed in meV/Å^2. Additionally, the number of hydroxyl groups per unit cell is listed, see Table S8 for the surface area of these unit cells.

Oxide	$\Delta\gamma_{\mathrm{ox-lat}}^{\mathrm{ox}}$	n / UC
O-α-SiO_2(0001)	272.03	2
O-α-Al_2O_3(0001)	414.39	3
2O-γ-Al_2O_3(110)	142.76	4
3O-γ-Al_2O_3(110)	222.33	6

S1.2 Further Analysis of the Results

- Figure S1 and S2 show adhesion energies formed with fcc(100)-surfaces as a function of oxygen adsorption energies on fcc(100)-surfaces.
- Table S2 lists adhesion energies from the literature for systems studied in this work.
- Figures S3 to S5 show the vdW-contribution to adhesion energies as evaluated through the D3-correction with both zero- and BJ-damping, where the latter has been evaluated in a single-point energy calculation on the structures that were all optimized with zero-damping D3 contribution.

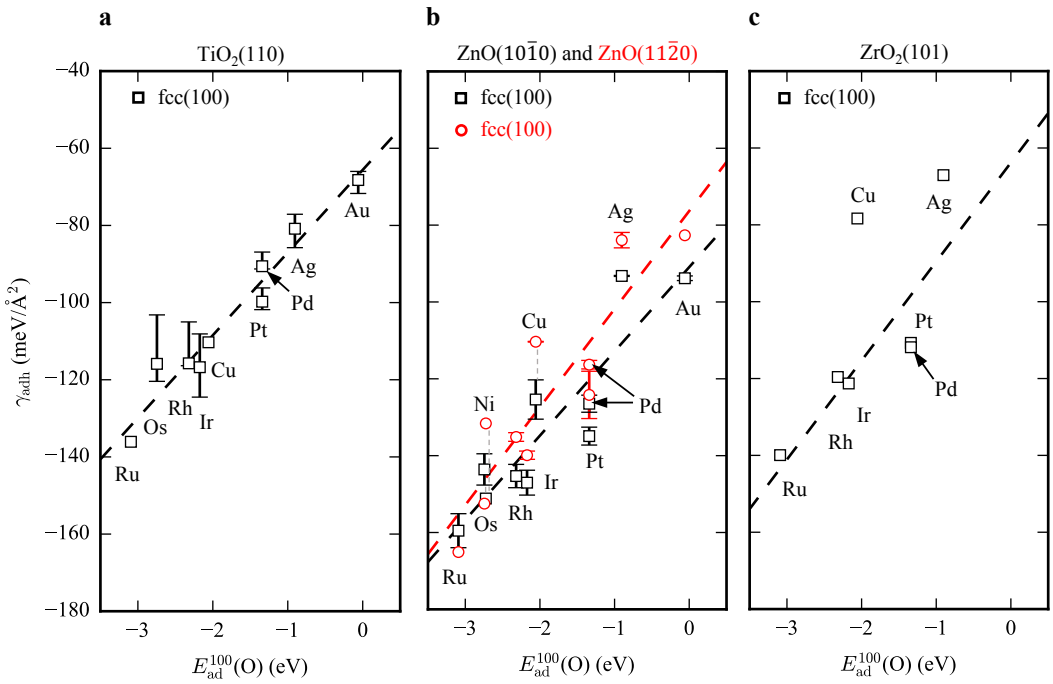

Fig. S1 Interfaces formed by stoichiometric oxide surfaces and fcc(111)- and fcc(100) metal surfaces. Adhesion energies for **a.** the 110-surface of rutile, **b.** the 10$\bar{1}$0- and 11$\bar{2}$0-surfaces of ZnO in wurtzite structure and **c.** the 101-surface of tetragonal ZrO_2 as a function of oxygen adsorption energies on clean fcc(100) metal surfaces.

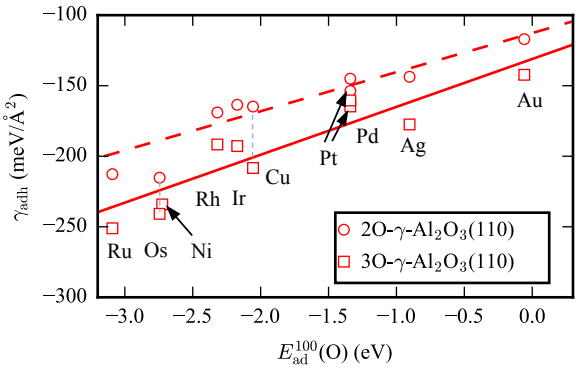

Fig. S2 Oxidized interfaces. Adhesion energies are shown as a function of oxygen adsorption energies on clean fcc(100) metal surfaces.

Table S2. Comparison of surface energies from the literature for systems studied in this work with the values obtained in this work.

metal	oxide	γ_{adh} (meV/Å^2)	ref
Au	TiO_2(110)	-34 to -44	ref. 17 of the main text
		-26 to -35	ref. 20 of the main text
Au(111)		-62 to -61	this work, Table S3
Au(100)		-68 to -70	this work, Table S3
Ag(111)	O-α-Al_2O_3(0001)	-253	ref. 26 of the main text
		-252 to -258	this work, Table S3

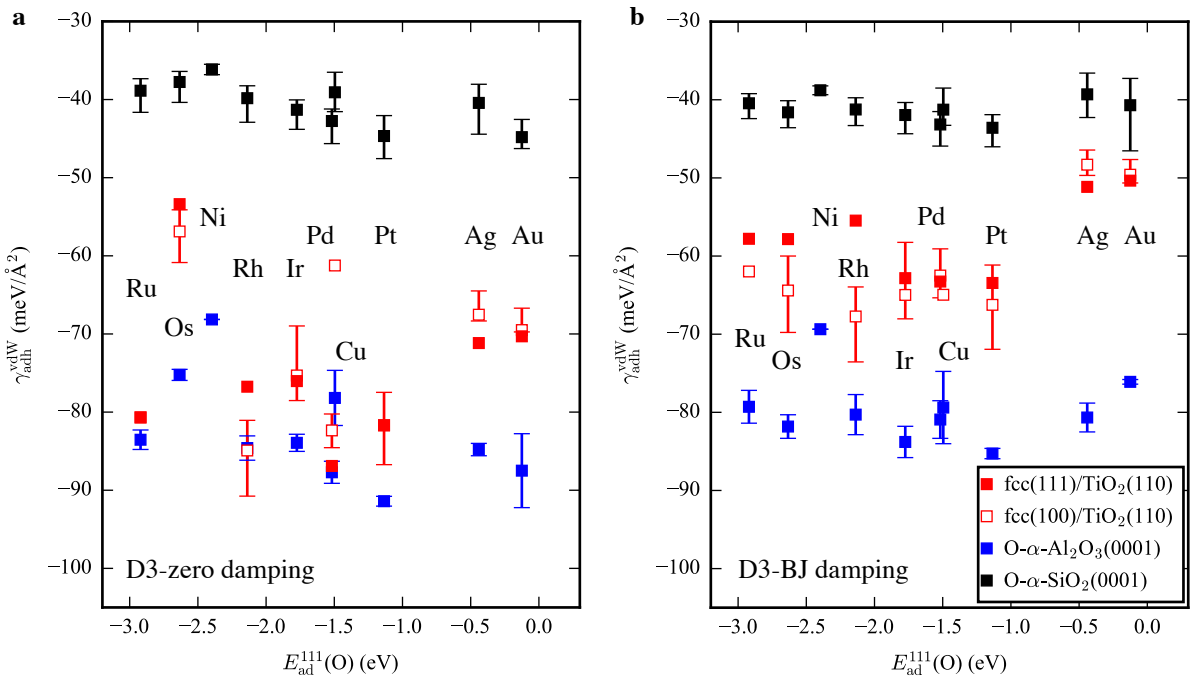

Fig. S3 Interfaces formed by oxygen-rich oxide surfaces that can be derived from hydroxylated surfaces and stoichiometric oxide surfaces. Van-der-Waals contributions with **a.** D3-zero damping and **b.** D3-BJ damping of adhesion energies are shown as a function of oxygen adsorption energies on clean fcc(111) metal surfaces. The van-der-Waals contributions of the adhesion energies were averaged over all computed supercells and the largest and smallest deviation within these individual calculations is indicated with error bars.

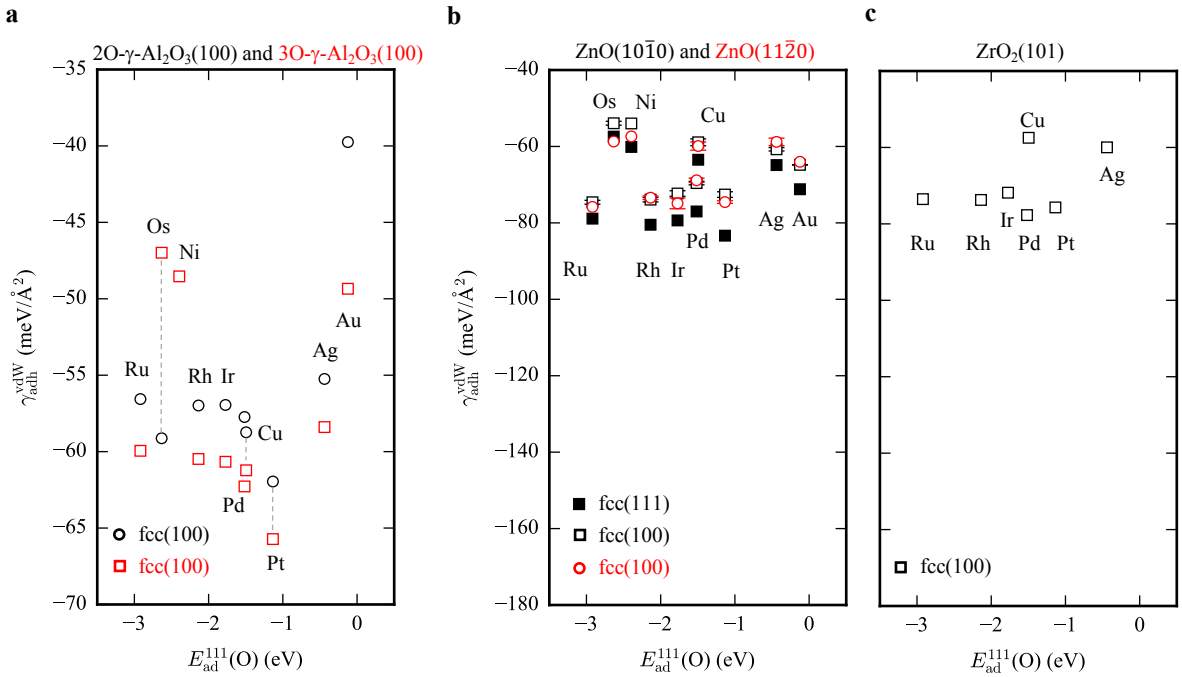

Fig. S4 VdW-contribution to adhesion energies. a. Van-der-Waals contribution with D3-zero damping to adhesion energies for the fcc(100)-surface of the hydroxylated γ-Al_2O_3 surfaces with two and three adsorbed water molecules per unit cell. **b.** Van-der-Waals contribution with D3-zero damping contribution of adhesion energies for the 10$\bar{1}$0- and 11$\bar{2}$0-surfaces of ZnO in wurtzite structure. **c.** Van-der-Waals contribution with D3-zero damping of adhesion energies for the 101-surface of tetragonal ZrO_2.

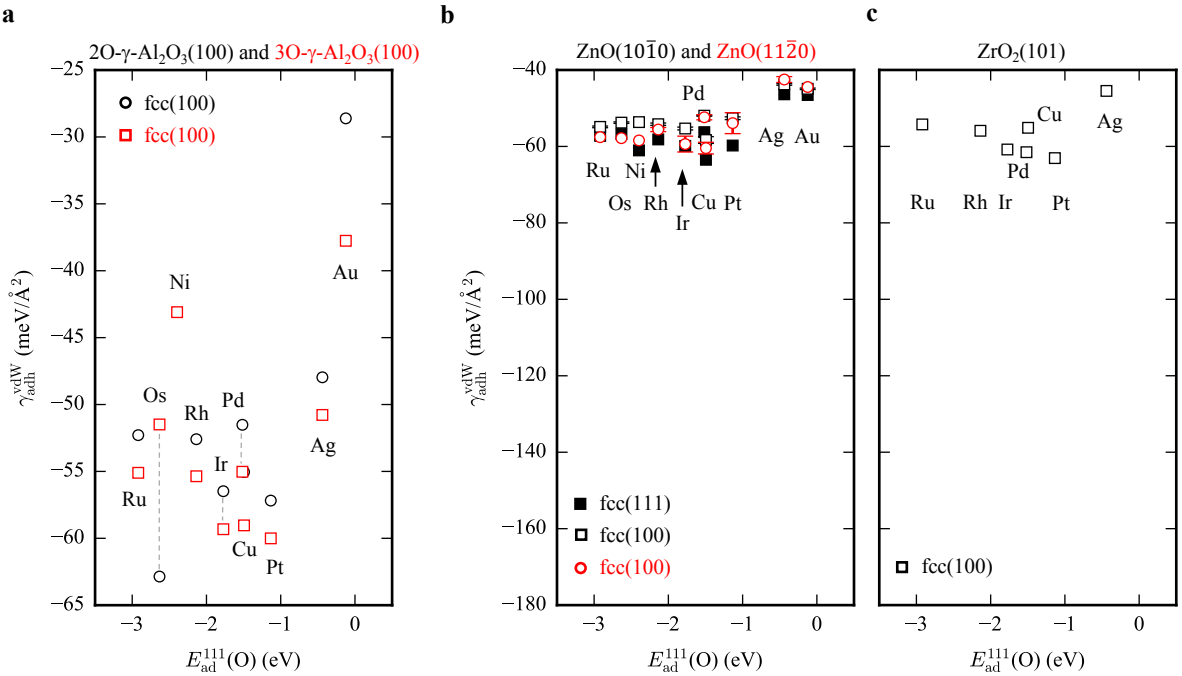

Fig. S5 VdW-contribution to adhesion energies. a. Van-der-Waals contribution with D3-BJ damping to adhesion energies between the fcc(100)-surface and the hydroxylated γ-Al_2O_3 surfaces with two and three adsorbed water molecules per unit cell. **b.** Van-der-Waals contribution with D3-BJ damping contribution of adhesion energies for the 10$\bar{1}$0- and 11$\bar{2}$0-

surfaces of ZnO in wurtzite structure. **c.** Van-der-Waals contribution with D3-BJ damping of adhesion energies for the 101-surface of tetragonal ZrO_2.

S1.3 Convergence of the number of oxid layers

To show the convergence of our results against the number of oxide layers we use the Pt/O-α-SiO_2(0001) interface as an example with various numbers of layers, ranging from 1 to 5. The first layer in the 1×1 O-α-SiO_2(0001) unit-cell consists of 4 SiO_2 groups. The following layers are containing each 3 SiO_2 groups to have the same hydrogen saturated oxygen atoms at the bottom. For the convergence test the complete structure is relaxed. We find that already after the first layer the number of oxide layers is converged and the adhesion energy varies maximal with 1.2 meV/ Å^2. The calculatued total energies and adhesion energies are given in Table S3. We calculated γ_{adh}=184.00 meV/Å^2 in the text. This is in good agreement with the results from the layer convergence.

Table S3. Convergence of the adhesion energy γ_{adh} in meV/Å^2 with the number of SiO_2 groups per unit cell N(SiO_2) using the example of the Pt/O-α-SiO_2(0001) interface.

N(SiO_2)	$E_{interface}$	E_{oxide}	E_{Metal}	$\Delta\gamma^{ox}_{ox-lat}$	γ_{adh}
4	-192.75	-125.17	-76.28	272.03	-181.30
7	-264.77	-197.19	-76.28	272.03	-180.94
10	-336.84	-269.24	-76.28	272.03	-182.15
13	-408.90	-341.32	-76.28	272.03	-181.45
16	-480.96	-413.36	-76.28	272.03	-182.16

S2 List of Calculated Properties

- Table S4 lists all computed adhesion energies.
- Table S5 lists oxygen adsorption energies used for the scaling relations.
- Table S6 lists the parameters and errors obtained for the scaling relations.
- Table S7 lists the metal-oxygen distances measured for interfaces with O-α-SiO_2(0001) and O-α-Al_2O_3(0001) and the derived bond-length criterion.
- Table S8 lists the obtained number of interfacial oxygen atoms using the criteria listed in Table S7.
- Table S9 lists the surface lattice constants of the oxide surfaces as well as the area of the unit cell.
- Table S10 lists the employed bulk lattice constants of the metals in fcc structure.
- Table S11 lists the strain on the oxide for all interfaces.
- Table S12 lists the vdW-interaction within bulk oxides and bulk metals.
- Table S13 lists the employed k-point sampling.
- Table S14 lists the total energies employed to compute adhesion energies as well as the employed surface areas.

Table S4a. Adhesion energies of O–α-SiO_2(0001) in meV/Å^2 as shown in Fig. 3.

Surface	O-α-SiO_2(0001)			O-α-Al_2O_3(0001)	
Metal	fcc(111)			fcc(111)	
Supercell	2×2	$(\sqrt{3}\times\sqrt{3})R30^c$	$(\sqrt{13}\times\sqrt{13})R14^c$	$(\sqrt{3}\times\sqrt{3})R30^c$	$(\sqrt{13}\times\sqrt{13})R14^c$
Ag	-219.96	-190.41	-195.88	-251.77	-258.07
Au	-164.07	-146.90	-149.18	-196.95	-216.91
Cu	-243.12	-215.14	-228.33	-282.91	-308.28
Ir	-235.13	-224.36	-235.70	-398.92	-348.53
Ni	-248.07	-224.90	-	-340.84	-
Pd	-211.86	-181.82	-198.75	-281.49	-286.48
Pt	-202.76	-184.00	-195.98	-315.45	-289.45
Os	-281.74	-249.65	-245.78	-460.47	-373.82
Rh	-255.89	-219.46	-234.45	-372.25	-345.01
Ru	-298.01	-268.43	-251.79	-441.62	-392.24

Table S4b. Adhesion energies in meV/Å^2 as shown in Fig. 4.

Surface	2O-γ-Al_2O_3(110)	3O-γ-Al_2O_3(110)	ZrO_2(101)
Metal	fcc(100)	fcc(100)	fcc(100)
Ag	-143.69	-177.48	-67.37
Au	-117.01	-142.27	-
Cu	-164.76	-208.34	-78.35
Ir	-163.51	-192.80	-121.29
Ni	-	-234.17	-
Pd	-153.71	-160.46	-111.85
Pt	-145.02	-164.71	-110.72
Os	-215.22	-240.84	-
Rh	-168.96	-191.66	-119.60
Ru	-212.72	-251.07	-139.93

Table S4c. Adhesion energies in meV/Å^2 as shown in Fig. 3.

Surface	$TiO_2(110)$				
Metal	fcc(100)				fcc(111)
Oxide supercell	2×1	3×1	4×1	1×2	3×5
Metal supercell	5×1	7×1	9×1	$(\sqrt{5}\times\sqrt{5})R27°$	$7\times3\sqrt{3}$
Ag	-75.95	-81.19	-81.67	-84.61	-73.52
Au	-64.74	-68.64	-69.07	-70.45	-61.48
Cu	-110.29	-	-	-	-
Ir	-108.99	-105.88	-126.74	-125.37	-93.54
Ni	-	-	-	-	-
Pd	-97.69	-98.26	-	-103.32	-99.01
Pt	-89.86	-91.93	-86.25	-94.24	-86.49
Os	-111.34	-107.72	-	-128.57	-81.45
Rh	-115.12	-105.62	-	-126.47	-118.41
Ru	-136.08	-	-	-187.68	-126.09

Table S4d. Adhesion energies in meV/Å^2 as shown in Fig. 4.

Surface	$ZnO(10\bar{1}0)$			$ZnO(11\bar{2}0)$	
Metal	fcc(100)		fcc(111)	fcc(100)	
Oxide supercell	4×1	5×1	3×1	1×1	2×3
Metal supercell	5×2	6×2	$2\sqrt{3}\times2$	2×2	$3\sqrt{2}\times4\sqrt{2}$
Ag	-93.35	-93.10	-91.34	-85.92	-81.91
Au	-93.23	-94.43	-89.60	-82.65	-
Cu	-120.27	-130.51	-136.76	-110.43	-110.27
Ir	-143.79	-150.27	-141.63	-140.96	-138.81
Ni	-151.16	-	-161.54	-131.61	-
Pd	-124.26	-128.70	-133.31	-115.21	-117.43
Pt	-132.58	-137.24	-137.33	-118.03	-130.35
Os	-139.51	-147.65	-121.79	-152.48	-
Rh	-142.27	-148.34	-148.25	-134.02	-136.27
Ru	-155.10	-163.96	-147.29	-165.09	-

Table S5. Oxygen adsorption energy on fcc(111) and fcc(100) metal surfaces with 1/9 (3×3) oxygen coverage.

Metal	fcc(111) 3×3	fcc(100) 3×3
Ag	-0.44	-0.90
Au	-0.12	-0.06
Cu	-1.49	-2.06
Ir	-1.77	-2.17
Ni	-2.40	-2.72
Pd	-1.52	-1.34
Pt	-1.13	-1.34
Os	-2.63	-2.74
Rh	-2.14	-2.32
Ru	-2.92	-3.09

Table S6. Obtained scaling parameters a_{ox} and b_{ox} and the mean absolute error (MAE) from Fig. 3 and Fig. 4 and number of interfacial oxygen atoms c_o, plotted in Fig. 4a, b. If c_o cannot be determent from the number of surface oxygens, the mean number of M-O bonds for all calculated metal/oxide interfaces is used. A bond counts as an M-O bound, if the M-O distance is smaller than the criterion given in Table S6.

Oxide surface	Metal surface	Metal supercell	a_{ox} (10^{-3} Å^{-2})	b_{ox} (meV/ Å^2)	MAE (meV/ Å^2)	c_o (nm^{-2})
O-α-SiO_2(0001)	fcc(111)	$(\sqrt{13}\times\sqrt{13})$R14°	36.75	-161.72	10.41	9.38
O-α-Al_2O_3(0001)	fcc(111)	$(\sqrt{13}\times\sqrt{13})$R14°	70.54	-208.26	19.23	15.12
2O-γ-Al_2O_3(110)	fcc(100)	3×3	28.95	-116.94	7.48	7.82
3O-γ-Al_2O_3(110)	fcc(100)	3×3	33.46	-139.65	15.55	9.87
TiO_2(110)	fcc(100)	7×1	23.54	-68.33	3.91	7.71
	fcc(111)	7×3	23.54	-60.30	3.91	5.14
ZnO(100)	fcc(100)	5×2	24.45	-92.96	6.27	5.78
	fcc(111)	2×2	24.45	-92.93	8.92	5.78
ZnO(110)	fcc(100)	2×2	27.76	-78.18	7.03	6.68
ZrO_2(101)	fcc(100)	3×3	26.30	-68.32	7.52	6.64

Table S7. Minimum and maximum M-O distance in Å for fcc(111) $\left(\sqrt{13}\times\sqrt{13}\right)R14°$/ O-α-$SiO_2$(0001) and fcc(111) $\left(\sqrt{13}\times\sqrt{13}\right)R14°$/ O-α-$Al_2O_3$(0001) and the derived, employed cut-off criterion.

Metal	O-α-SiO_2(0001)		O-α-Al_2O_3(0001)		Employed cut-off criterion
	d_{min}	d_{max}	d_{min}	d_{max}	
Ag	2.15	2.22	2.07	2.30	2.60
Au	2.07	2.23	2.02	2.19	2.49
Cu	1.85	2.05	1.85	2.01	2.31
Ir	1.95	2.13	1.96	2.23	2.53
Ni	1.85	1.91	1.80	1.89	2.19
Pd	1.97	2.10	1.97	2.14	2.44
Pt	1.99	2.12	1.95	2.12	2.42
Os	1.95	2.15	1.97	2.20	2.50
Rh	1.94	2.07	1.94	2.11	2.41
Ru	1.94	2.10	1.95	2.12	2.42

Table S8. Obtained number of interfacial oxygen atoms N_O per calculated supercell for all metal/interface combinations with the criterion mentioned above (Table S7). fcc(111) $\left(\sqrt{13}\times\sqrt{13}\right)R14°$/ O-α-$SiO_2$(0001) and fcc(111) $\left(\sqrt{13}\times\sqrt{13}\right)R14°$/ O-α-$Al_2O_3$(0001) are used. The column labeled ideal gives the number of oxygen atoms that one could derive from the number of surface oxygen atoms of the clean oxide surface. Where this number is close to the actual number, it was used as the actual concentration (last column).

Oxide surface	Metal surface	Metal supercell	Ag	Au	Cu	Ir	Ni	Pd	Pt	Os	Rh	Ru	ideal	employed value
O-α-SiO_2(0001)	fcc(111)	$\sqrt{13}$	8	8	8	8	8	8	8	8	8	8	8	8
O-α-Al_2O_3(0001)	fcc(111)	$\sqrt{13}$	12	12	12	12	12	12	12	12	12	12	12	12
2O-γ-Al_2O_3(110)	fcc(100)	3×3	5	5	5	5	-	5	5	-	5	7	2	5.250
3O-γ-Al_2O_3(110)	fcc(100)	3×3	8	-	8	6	7	6	6	-	6	6	3	6.625
TiO_2(110)	fcc(100)	7×1	3	2	-	3	-	3	3	3	3	3	3	3
	fcc(111)	7×3	15	8	-	15	-	15	14	15	15	16	15	15
ZnO(10$\bar{1}$0)	fcc(100)	5×2	4	2	4	4	4	4	4	4	4	4	4	4
	fcc(111)	2×2	3	1	3	3	3	3	3	3	3	3	3	3
ZnO(11$\bar{2}$0)	fcc(100)	2×2	2	0	2	2	2	2	2	2	2	2	2	2
ZrO_2(101)	fcc(100)	3×3	11	-	9	16	-	14	14	-	14	18	9	13.714

Table S9. Unit cell surface area in Å^2 of the oxide surfaces and the surface lattice parameters.

Oxide surface	Surface area	Lattice parameter	
		a	b
O-α-SiO_2(0001)	21.33	4.962	
O-α-Al_2O_3(0001)	19.85	4.787	
2O-γ-Al_2O_3(110)	67.11	8.035	8.352
3O-γ-Al_2O_3(110)	67.11	8.035	8.352
TiO_2(110)	19.45	6.569	2.960
ZnO($10\bar{1}0$)	17.30	3.274	5.283
ZnO($11\bar{2}0$)	29.96	5.671	5.283
ZrO_2(101)	22.95	6.361	3.608

Table S10. PBE-D3 optimized metal bulk lattice parameter.

Metal	Lattice parameter
Ag	2.881 Å
Au	2.899 Å
Cu	2.524 Å
Ir	2.715 Å
Ni	2.454 Å
Pd	2.748 Å
Pt	2.770 Å
Os	2.708 Å
Rh	2.678 Å
Ru	2.666 Å

Table S11a. Strain of metal/oxide interface in %.

Surface	O-α-SiO_2(0001)			O-α-Al_2O_3(0001)	
Metal	fcc(111)			fcc(111)	
Supercell	2×2	$(\sqrt{3}\times\sqrt{3})R30°$	$(\sqrt{13}\times\sqrt{13})R14°$	$(\sqrt{3}\times\sqrt{3})R30°$	$(\sqrt{13}\times\sqrt{13})R14°$
Ag	16.12	0.54	4.66	4.22	8.48
Au	16.85	1.19	5.32	4.89	9.17
Cu	1.73	-11.91	-8.30	-8.69	-4.95
Ir	9.43	-5.22	-1.36	-1.75	2.25
Ni	-1.09	-14.35	-10.84	-11.22	-7.58
Pd	10.76	-4.07	-0.16	-0.56	3.49
Pt	11.65	-3.28	0.65	0.25	4.33
Os	9.15	-5.46	-1.60	-2.01	1.99
Rh	7.94	-6.53	-2.72	-3.11	0.84
Ru	7.46	-6.93	-3.13	-3.53	0.41

Table S11b. Strain of metal/oxide interfaces in %.

Surface	2O-γ-Al_2O_3(110)		3O-γ-Al_2O_3(110)		ZrO_2(101)	
Metal	fcc(100)		fcc(100)		fcc(100)	
Metal supercell	3×3		3×3		7×4	
	a	b	a	b	a	b
Ag	3.48	7.57	3.48	7.57	5.68	6.47
Au	4.13	8.24	4.13	8.24	6.34	7.13
Cu	-9.34	-5.76	-9.34	-5.76	-7.41	-6.73
Ir	-2.48	1.37	-2.48	1.37	-0.41	0.33
Ni	-11.85	-8.38	-11.85	-8.38	-9.98	-9.31
Pd	-1.29	2.60	-1.29	2.60	0.80	1.55
Pt	-0.50	3.42	-0.50	3.42	1.61	2.37
Os	-2.73	1.11	-2.73	1.11	-0.67	0.07
Rh	-3.81	-0.01	-3.81	-0.01	-1.77	-1.03
Ru	-4.24	-0.46	-4.24	-0.46	-2.21	-1.48

Table S11c. Strain of metal/oxide interfaces in %.

Surface	TiO_2(110)									
Metal	fcc(100)								fcc(111)	
Oxide supercell	2×1		3×1		4×1		1×2		3×5	
Metal supercell	5×1		7×1		9×1		$(\sqrt{5}\times\sqrt{5})R27°$		$7\times3\sqrt{3}$	
	a	b	a	b	a	b	a	b	a	b
Ag	9.64	-2.67	2.33	-2.67	-1.32	-2.67	-1.95	8.80	2.33	1.13
Au	10.33	-2.06	2.97	-2.06	-0.70	-2.06	-1.33	9.49	2.97	1.78
Cu	-3.94	-14.73	-10.35	-14.73	-13.55	-14.73	-14.09	-4.67	-10.35	-11.40
Ir	3.33	-8.28	-3.56	-8.28	-7.01	-8.28	-7.58	2.55	-3.56	-4.67
Ni	-6.61	-17.09	-12.83	-17.09	-15.95	-17.09	-16.47	-7.31	-12.83	-13.85
Pd	4.58	-7.16	-2.39	-7.16	-5.88	-7.16	-6.46	3.80	-2.39	-3.51
Pt	5.42	-6.42	-1.61	-6.42	-5.12	-6.42	-5.69	4.64	-1.61	-2.72
Os	3.06	-8.51	-3.81	-8.51	-7.25	-8.51	-7.81	2.30	-3.81	-4.91
Rh	1.92	-9.53	-4.88	-9.53	-8.27	-9.53	-8.85	1.14	-4.88	-5.99
Ru	1.46	-9.93	-5.30	-9.93	-8.68	-9.93	-9.24	0.71	-5.30	-6.39

Table S11d. Strain of metal/oxide interfaces in %.

Surface	$ZnO(10\bar{1}0)$						$ZnO(11\bar{2}0)$			
Metal	fcc(100)				fcc(111)		fcc(100)			
Oxide supercell	4×1		5×1		3×1		1×1		2×3	
Metal supercell	5×2		6×2		$2\sqrt{3}\times2$		2×2		$3\sqrt{2}\times4\sqrt{2}$	
	a	b	a	b	a	b	a	b	a	b
Ag	10.00	9.07	5.60	9.07	1.59	9.07	1.60	9.07	7.77	2.83
Au	10.68	9.75	6.26	9.75	2.24	9.75	2.24	9.75	8.44	3.47
Cu	-3.63	-4.45	-7.49	-4.45	-11.00	-4.45	-10.99	-4.45	-5.59	-9.91
Ir	3.66	2.78	-0.49	2.78	-4.24	2.78	-4.25	2.78	1.56	-3.10
Ni	-6.31	-7.10	-10.05	-7.10	-13.46	-7.10	-13.45	-7.10	-8.20	-12.41
Pd	4.92	4.03	0.72	4.03	-3.07	4.03	-3.09	4.03	2.79	-1.92
Pt	5.76	4.86	1.53	4.86	-2.28	4.86	-2.31	4.86	3.62	-1.13
Os	3.39	2.52	-0.75	2.52	-4.48	2.52	-4.50	2.52	1.30	-3.35
Rh	2.24	1.38	-1.84	1.38	-5.56	1.38	-5.55	1.38	0.17	-4.42
Ru	1.79	0.93	-2.28	0.93	-5.97	0.93	-5.98	0.93	-0.27	-4.84

Table S12. Van-der-Waals energy with zero damping per volume for bulk oxides and van-der-Waals energy with zero damping per atom of bulk metals.

Oxide	E_{vdW}/V (meV/ Å^3)	Metal	E_{vdW} (eV)
α-SiO_2	-7.509	Ag	-0.505
α–Al_2O_3	-18.115	Au	-0.670
γ-Al_2O_3	-15.773	Cu	-0.525
TiO_2	-16.581	Ir	-0.719
ZnO	-16.606	Ni	-0.413
ZrO_2	-16.127	Pd	-0.592
		Pt	-0.783
		Os	-0.595
		Rh	-0.587
		Ru	-0.563

Table S13. Surface dependent Γ−centered k-point sampling.

Oxide surface	Metal surface	Metall supercell	K-points
O-α-SiO_2(0001)	fcc(111)	2×2	(8,8,1)
		$(\sqrt{3}\times\sqrt{3})R30°$	(8,8,1)
		$(\sqrt{13}\times\sqrt{13})R14°$	(3,3,1)
O-α-Al_2O_3(0001)	fcc(111)	$(\sqrt{3}\times\sqrt{3})R30°$	(8,8,1)
		$(\sqrt{13}\times\sqrt{13})R14°$	(3,3,1)
2O-γ-Al_2O_3(110)	fcc(100)	3×3	(4,4,1)
3O-γ-Al_2O_3(110)	fcc(100)	3×3	(4,4,1)
TiO_2(110)	fcc(100)	5×1	(2,10,1)
		7×1	(2,10,1)
		9×1	(1,10,1)
		$(\sqrt{5}\times\sqrt{5})R27°$	(5,5,1)
	fcc(111)	$7\times3\sqrt{3}$	(2,2,1)
ZnO$(10\bar{1}0)$	fcc(100)	5×2	(2,5,1)
		6×2	(2,5,1)
	fcc(111)	$2\sqrt{3}\times2$	(3,6,1)
ZnO$(11\bar{2}0)$	fcc(100)	2×2	(6,6,1)
		$3\sqrt{2}\times4\sqrt{2}$	(3,2,1)
ZrO_2(101)	fcc(100)	7×4	(2,3,1)

Table S14. Interface energy, oxide energy, metal energy and surface area in Å^2 for all calculated metal/oxide structures. In the case of the hydroxylated oxide, the surface area of the strain-free oxide surface is used and the number of hydroxyl groups per supercell and the stability difference between hydroxylated and oxidized surfaces per supercell given. For the stoichiometric interfaces the surface area depending on the metal lattice constant is given.

Surface	$E_{Interface}$	E_{Oxide}	E_{Metal}	Area	N_{OH}	$\Delta\gamma^{ox}_{ox-lat}$
2O-γ-Al_2O_3(110)/fcc(100)_3x3/Ag	-805.82	-687.91	-131.37	67.11	4	142.76
2O-γ-Al_2O_3(110)/fcc(100)_3x3/Au	-830.71	-686.26	-159.70	67.11	4	142.76
2O-γ-Al_2O_3(110)/fcc(100)_3x3/Cu	-840.04	-678.10	-173.98	67.11	4	142.76
2O-γ-Al_2O_3(110)/fcc(100)_3x3/Ir	-1080.43	-694.35	-398.21	67.11	4	142.76
2O-γ-Al_2O_3(110)/fcc(100)_3x3/Os	-1173.77	-694.27	-488.16	67.11	4	142.76
2O-γ-Al_2O_3(110)/fcc(100)_3x3/Pd	-922.69	-694.33	-241.15	67.11	4	142.76
2O-γ-Al_2O_3(110)/fcc(100)_3x3/Pt	-965.33	-693.87	-284.83	67.11	4	142.76
2O-γ-Al_2O_3(110)/fcc(100)_3x3/Rh	-1008.84	-693.48	-327.12	67.11	4	142.76
2O-γ-Al_2O_3(110)/fcc(100)_3x3/Ru	-1089.56	-693.02	-405.37	67.11	4	142.76
3O-γ-Al_2O_3(110)/fcc(100)_3x3/Ag	-813.09	-705.01	-131.37	67.11	6	222.33
3O-γ-Al_2O_3(110)/fcc(100)_3x3/Au	-837.54	-703.49	-159.70	67.11	6	222.33
3O-γ-Al_2O_3(110)/fcc(100)_3x3/Cu	-846.80	-694.04	-173.98	67.11	6	222.33
3O-γ-Al_2O_3(110)/fcc(100)_3x3/Ir	-1086.75	-710.81	-398.21	67.11	6	222.33
3O-γ-Al_2O_3(110)/fcc(100)_3x3/Ni	-904.77	-680.24	-244.02	67.11	6	222.33

3O-γ-Al_2O_3(110)/fcc(100)_3x3/Os	-1179.85	-710.73	-488.16	67.11	6	222.33
3O-γ-Al_2O_3(110)/fcc(100)_3x3/Pd	-927.59	-710.87	-241.15	67.11	6	222.33
3O-γ-Al_2O_3(110)/fcc(100)_3x3/Pt	-971.15	-710.47	-284.83	67.11	6	222.33
3O-γ-Al_2O_3(110)/fcc(100)_3x3/Rh	-1014.65	-709.87	-327.12	67.11	6	222.33
3O-γ-Al_2O_3(110)/fcc(100)_3x3/Ru	-1096.39	-709.37	-405.37	67.11	6	222.33
O-α-Al_2O_3(0001)/fcc(111)_sqrt13/Ag	-1127.44	-1070.81	-109.60	79.38	12	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt13/Au	-1145.77	-1067.55	-134.45	79.38	12	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt13/Cu	-1173.06	-1076.28	-145.76	79.38	12	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt13/Ir	-1382.47	-1089.65	-338.61	79.38	12	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt13/Os	-1466.95	-1089.91	-420.82	79.38	12	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt13/Pd	-1240.33	-1087.75	-203.29	79.38	12	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt13/Pt	-1276.08	-1085.67	-240.88	79.38	12	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt13/Rh	-1321.69	-1090.47	-277.28	79.38	12	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt13/Ru	-1395.04	-1090.45	-346.90	79.38	12	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt3/Ag	-293.12	-271.55	-34.93	19.85	3	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt3/Au	-299.26	-271.08	-42.64	19.85	3	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt3/Cu	-295.38	-261.80	-46.32	19.85	3	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt3/Ir	-368.48	-271.99	-106.94	19.85	3	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt3/Ni	-307.72	-254.10	-65.22	19.85	3	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt3/Os	-394.30	-271.86	-131.66	19.85	3	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt3/Pd	-323.97	-272.45	-64.30	19.85	3	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt3/Pt	-336.78	-272.61	-76.28	19.85	3	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt3/Rh	-347.52	-271.06	-87.44	19.85	3	414.39
O-α-Al_2O_3(0001)/fcc(111)_sqrt3/Ru	-369.79	-270.68	-108.71	19.85	3	414.39
O-α-SiO_2(0001)/fcc(111)_2x2/Ag	-249.94	-211.27	-46.54	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_2x2/Au	-258.28	-210.46	-56.89	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_2x2/Cu	-275.46	-221.10	-61.74	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_2x2/Ir	-352.48	-217.47	-142.55	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_2x2/Ni	-300.99	-221.27	-86.99	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_2x2/Os	-386.66	-217.67	-175.54	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_2x2/Pd	-294.18	-216.42	-85.79	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_2x2/Pt	-309.08	-215.66	-101.66	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_2x2/Rh	-327.95	-218.52	-116.54	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_2x2/Ru	-357.54	-218.81	-144.93	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt13/Ag	-956.92	-880.85	-109.60	85.3	8	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt13/Au	-976.78	-879.85	-134.45	85.3	8	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt13/Cu	-983.28	-868.28	-145.76	85.3	8	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt13/Ir	-1192.90	-884.43	-338.61	85.3	8	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt13/Os	-1275.85	-884.31	-420.82	85.3	8	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt13/Pd	-1054.86	-884.86	-203.29	85.3	8	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt13/Pt	-1092.00	-884.64	-240.88	85.3	8	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt13/Rh	-1130.26	-883.23	-277.28	85.3	8	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt13/Ru	-1200.83	-882.69	-346.90	85.3	8	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt3/Ag	-247.64	-221.21	-34.93	21.33	2	272.03

O-α-SiO_2(0001)/fcc(111)_sqrt3/Au	-254.31	-221.10	-42.64	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt3/Cu	-250.37	-212.02	-46.32	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt3/Ir	-318.84	-219.67	-106.94	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt3/Ni	-264.58	-207.13	-65.22	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt3/Os	-343.95	-219.52	-131.66	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt3/Pd	-275.90	-220.29	-64.30	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt3/Pt	-288.26	-220.62	-76.28	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt3/Rh	-298.29	-218.74	-87.44	21.33	2	272.03
O-α-SiO_2(0001)/fcc(111)_sqrt3/Ru	-320.28	-218.41	-108.71	21.33	2	272.03
TiO_2(110)/fcc(100)_5x1/Ag	-466.67	-422.60	-40.92	41.49		
TiO_2(110)/fcc(100)_5x1/Au	-474.99	-422.25	-50.01	42.01		
TiO_2(110)/fcc(100)_5x1/Cu	-457.77	-399.84	-54.42	31.85		
TiO_2(110)/fcc(100)_5x1/Ir	-550.78	-420.85	-125.91	36.86		
TiO_2(110)/fcc(100)_5x1/Os	-579.13	-420.51	-154.53	36.68		
TiO_2(110)/fcc(100)_5x1/Pd	-501.99	-422.11	-76.19	37.76		
TiO_2(110)/fcc(100)_5x1/Pt	-515.71	-422.65	-89.61	38.38		
TiO_2(110)/fcc(100)_5x1/Rh	-526.42	-418.68	-103.62	35.85		
TiO_2(110)/fcc(100)_5x1/Ru	-550.78	-417.83	-128.11	35.54		
TiO_2(110)/fcc(100)_7x1/Ag	-699.77	-637.94	-57.12	58.08		
TiO_2(110)/fcc(100)_7x1/Au	-711.88	-637.91	-69.94	58.82		
TiO_2(110)/fcc(100)_7x1/Ir	-807.52	-625.88	-176.17	51.60		
TiO_2(110)/fcc(100)_7x1/Os	-846.60	-624.87	-216.20	51.35		
TiO_2(110)/fcc(100)_7x1/Pd	-742.09	-630.28	-106.61	52.86		
TiO_2(110)/fcc(100)_7x1/Pt	-763.08	-632.69	-125.45	53.73		
TiO_2(110)/fcc(100)_7x1/Rh	-769.98	-619.60	-145.07	50.19		
TiO_2(110)/fcc(100)_9x1/Ag	-929.64	-849.85	-73.68	74.68		
TiO_2(110)/fcc(100)_9x1/Au	-945.98	-850.71	-90.05	75.62		
TiO_2(110)/fcc(100)_9x1/Ir	-1059.35	-824.69	-226.25	66.34		
TiO_2(110)/fcc(100)_9x1/Pt	-1004.17	-836.70	-161.51	69.08		
TiO_2(110)/fcc(100)_sqrt5/Ag	-465.16	-420.72	-40.93	41.49		
TiO_2(110)/fcc(100)_sqrt5/Au	-473.10	-420.24	-49.91	42.01		
TiO_2(110)/fcc(100)_sqrt5/Ir	-551.41	-421.10	-125.69	36.86		
TiO_2(110)/fcc(100)_sqrt5/Os	-579.98	-420.81	-154.46	36.68		
TiO_2(110)/fcc(100)_sqrt5/Pd	-502.18	-422.16	-76.11	37.76		
TiO_2(110)/fcc(100)_sqrt5/Pt	-515.73	-422.54	-89.58	38.38		
TiO_2(110)/fcc(100)_sqrt5/Rh	-527.18	-419.13	-103.52	35.85		
TiO_2(110)/fcc(100)_sqrt5/Ru	-553.20	-418.37	-128.16	35.54		
TiO_2(110)/fcc(111)_7x3sqrt3/Ag	-3564.15	-3187.96	-354.01	301.80		
TiO_2(110)/fcc(111)_7x3sqrt3/Au	-3637.90	-3184.56	-434.55	305.63		
TiO_2(110)/fcc(111)_7x3sqrt3/Ir	-4285.48	-3165.96	-1094.43	268.13		
TiO_2(110)/fcc(111)_7x3sqrt3/Os	-4543.25	-3162.50	-1359.01	266.81		
TiO_2(110)/fcc(111)_7x3sqrt3/Pd	-3863.22	-3179.69	-656.33	274.67		
TiO_2(110)/fcc(111)_7x3sqrt3/Pt	-3988.05	-3186.11	-777.80	279.18		
TiO_2(110)/fcc(111)_7x3sqrt3/Rh	-4071.31	-3144.78	-895.65	260.79		

TiO_2(110)/fcc(111)_7x3sqrt3/Ru	-4291.52	-3137.02	-1121.89	258.56
ZnO(10$\bar{1}$0)/fcc(100)_5x2/Ag	-367.49	-277.91	-81.83	82.97
ZnO(10$\bar{1}$0)/fcc(100)_5x2/Au	-384.44	-276.58	-100.03	84.03
ZnO(10$\bar{1}$0)/fcc(100)_5x2/Cu	-402.20	-285.70	-108.84	63.69
ZnO(10$\bar{1}$0)/fcc(100)_5x2/Ir	-548.95	-286.52	-251.83	73.72
ZnO(10$\bar{1}$0)/fcc(100)_5x2/Ni	-445.00	-281.83	-154.07	60.21
ZnO(10$\bar{1}$0)/fcc(100)_5x2/Os	-606.01	-286.72	-309.06	73.36
ZnO(10$\bar{1}$0)/fcc(100)_5x2/Pd	-447.18	-285.42	-152.37	75.51
ZnO(10$\bar{1}$0)/fcc(100)_5x2/Pt	-473.85	-284.47	-179.21	76.75
ZnO(10$\bar{1}$0)/fcc(100)_5x2/Rh	-504.81	-287.39	-207.22	71.70
ZnO(10$\bar{1}$0)/fcc(100)_5x2/Ru	-554.80	-287.55	-256.22	71.09
ZnO(10$\bar{1}$0)/fcc(100)_6x2/Ag	-459.13	-351.82	-98.04	99.57
ZnO(10$\bar{1}$0)/fcc(100)_6x2/Au	-480.03	-350.47	-120.04	100.83
ZnO(10$\bar{1}$0)/fcc(100)_6x2/Cu	-493.82	-353.44	-130.40	76.43
ZnO(10$\bar{1}$0)/fcc(100)_6x2/Ir	-674.34	-359.15	-301.89	88.46
ZnO(10$\bar{1}$0)/fcc(100)_6x2/Os	-742.71	-359.22	-370.49	88.03
ZnO(10$\bar{1}$0)/fcc(100)_6x2/Pd	-552.88	-358.47	-182.74	90.62
ZnO(10$\bar{1}$0)/fcc(100)_6x2/Pt	-585.62	-357.78	-215.20	92.10
ZnO(10$\bar{1}$0)/fcc(100)_6x2/Rh	-620.74	-359.36	-248.62	86.04
ZnO(10$\bar{1}$0)/fcc(100)_6x2/Ru	-680.65	-359.29	-307.38	85.30
ZnO(10$\bar{1}$0)/fcc(111)_2sqrt3x2/Ag	-285.25	-212.60	-67.40	57.49
ZnO(10$\bar{1}$0)/fcc(111)_2sqrt3x2/Au	-300.07	-211.99	-82.86	58.22
ZnO(10$\bar{1}$0)/fcc(111)_2sqrt3x2/Cu	-304.39	-208.72	-89.64	44.13
ZnO(10$\bar{1}$0)/fcc(111)_2sqrt3x2/Ir	-430.54	-214.91	-208.40	51.07
ZnO(10$\bar{1}$0)/fcc(111)_2sqrt3x2/Ni	-337.23	-203.49	-127.00	41.72
ZnO(10$\bar{1}$0)/fcc(111)_2sqrt3x2/Os	-480.01	-214.87	-258.95	50.82
ZnO(10$\bar{1}$0)/fcc(111)_2sqrt3x2/Pd	-346.99	-214.96	-125.06	52.32
ZnO(10$\bar{1}$0)/fcc(111)_2sqrt3x2/Pt	-370.39	-214.85	-148.24	53.18
ZnO(10$\bar{1}$0)/fcc(111)_2sqrt3x2/Rh	-392.49	-214.53	-170.59	49.67
ZnO(10$\bar{1}$0)/fcc(111)_2sqrt3x2/Ru	-435.37	-214.33	-213.79	49.25
ZnO(11$\bar{2}$0)/fcc(100)_2x2/Ag	-104.18	-68.67	-32.66	33.19
ZnO(11$\bar{2}$0)/fcc(100)_2x2/Au	-111.21	-68.47	-39.96	33.61
ZnO(11$\bar{2}$0)/fcc(100)_2x2/Cu	-114.67	-68.38	-43.48	25.48
ZnO(11$\bar{2}$0)/fcc(100)_2x2/Ir	-174.30	-69.60	-100.54	29.49
ZnO(11$\bar{2}$0)/fcc(100)_2x2/Ni	-131.89	-67.14	-61.58	24.09
ZnO(11$\bar{2}$0)/fcc(100)_2x2/Os	-197.50	-69.61	-123.42	29.34
ZnO(11$\bar{2}$0)/fcc(100)_2x2/Pd	-133.93	-69.55	-60.90	30.21
ZnO(11$\bar{2}$0)/fcc(100)_2x2/Pt	-144.85	-69.47	-71.76	30.70
ZnO(11$\bar{2}$0)/fcc(100)_2x2/Rh	-156.27	-69.58	-82.85	28.68
ZnO(11$\bar{2}$0)/fcc(100)_2x2/Ru	-176.72	-69.55	-102.47	28.43
ZnO(11$\bar{2}$0)/fcc(100)_3sqrt2x4sqrt2/Ag	-626.06	-413.22	-196.53	199.14
ZnO(11$\bar{2}$0)/fcc(100)_3sqrt2x4sqrt2/Cu	-687.49	-409.67	-260.97	152.87
ZnO(11$\bar{2}$0)/fcc(100)_3sqrt2x4sqrt2/Ir	-1046.37	-418.15	-603.66	176.92
ZnO(11$\bar{2}$0)/fcc(100)_3sqrt2x4sqrt2/Pd	-804.54	-417.95	-365.31	181.23

ZnO(11$\bar{2}$0)/fcc(100)_3sqrt2x4sqrt2/Pt	-871.45	-417.57	-429.87	184.21
ZnO(11$\bar{2}$0)/fcc(100)_3sqrt2x4sqrt2/Rh	-938.57	-417.82	-497.30	172.08
ZrO_2(101)/fcc(100)_7x4/Ag	-2288.87	-2044.13	-229.09	232.33
ZrO_2(101)/fcc(100)_7x4/Cu	-2376.37	-2057.80	-304.59	178.34
ZrO_2(101)/fcc(100)_7x4/Ir	-2799.18	-2070.05	-704.09	206.40
ZrO_2(101)/fcc(100)_7x4/Pd	-2517.29	-2067.45	-426.20	211.44
ZrO_2(101)/fcc(100)_7x4/Pt	-2590.35	-2064.62	-501.94	214.91
ZrO_2(101)/fcc(100)_7x4/Rh	-2676.26	-2072.10	-580.15	200.76
ZrO_2(101)/fcc(100)_7x4/Ru	-2817.53	-2072.29	-717.39	199.04

S3 Adhesion energies with oxide lattice constant

- Figure S6 shows the absolute change in adhesion energy when using either the metal lattice constans or the oxide lattice constant for the unit cell as a function of the absolute maximum strain of the metal/oxide interface.
- Table S15 lists the metal/oxide interfaces, corresponding adhesion energies when using either the metal lattice constant or the oxide lattice constant and the change in adhesion energy.
- Table S16 lists the total energies used to calculate the adhesion energies in Table S15 in the case of using the oxide lattice constant.

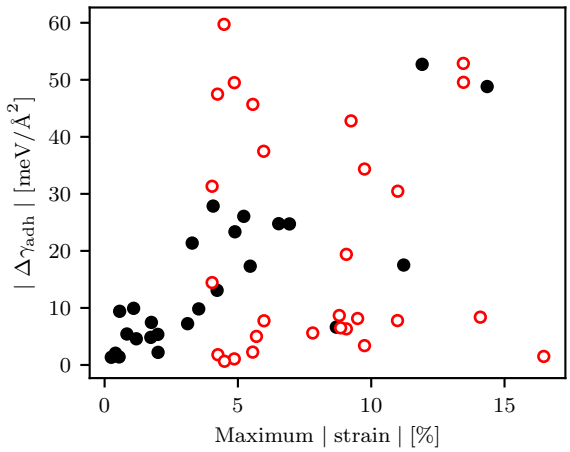

Figure S6. Absolute change in the adhesion energy when using either the metal lattice constant or the oxide lattice constant as a function of the absolute maximum strain of the metal/oxide interface. The black circles denote for symmetric strain (α-SiO_2 and α- Al_2O_3) and the red, empty circles asymmetric strain on the unit cell. In the case of asymmetric strain the absolute maximum strain is used. The corresponding interfaces and values are shown in Table S15.

Table S15. Adhesion energies in meV/ Å^2 with adjusting the metal to the oxide lattice constant $\gamma_{\mathrm{adh}}^{\mathrm{oxide-lattice}}$ for selected metal/oxide interfaces and comparison to the corresponding interfaces in the metal lattice constant $\gamma_{\mathrm{adh}}^{\mathrm{metal-lattice}}$. The change in the adhesion energy $\Delta\gamma_{\mathrm{adh}} = \gamma_{\mathrm{adh}}^{\mathrm{metal-lattice}} - \gamma_{\mathrm{adh}}^{\mathrm{oxide-lattice}}$. The strain in % is the absolute maximum strain of the metal/oxide interface.

Surface	$\gamma_{\mathrm{adh}}^{\mathrm{oxide-lattice}}$	$\gamma_{\mathrm{adh}}^{\mathrm{metal-lattice}}$	$\Delta\gamma_{\mathrm{adh}}$	Strain
O-a-Al2O3(0001)/fcc(111)_sqrt3/Ag	-238.68	-251.77	-13.09	4.22

O-a-Al2O3(0001)/fcc(111)_sqrt3/Au	-173.60	-196.95	-23.35	4.89
O-a-Al2O3(0001)/fcc(111)_sqrt3/Cu	-289.54	-282.91	6.63	8.69
O-a-Al2O3(0001)/fcc(111)_sqrt3/Ir	-406.39	-398.92	7.46	1.75
O-a-Al2O3(0001)/fcc(111)_sqrt3/Ni	-358.36	-340.84	17.52	11.22
O-a-Al2O3(0001)/fcc(111)_sqrt3/Os	-469.88	-460.47	9.41	0.56
O-a-Al2O3(0001)/fcc(111)_sqrt13/Os	-368.46	-373.82	-5.36	1.99
O-a-Al2O3(0001)/fcc(111)_sqrt3/Pd	-282.85	-281.49	1.35	0.25
O-a-Al2O3(0001)/fcc(111)_sqrt3/Pt	-313.24	-315.45	-2.21	2.01
O-a-Al2O3(0001)/fcc(111)_sqrt3/Rh	-379.49	-372.25	7.24	3.11
O-a-Al2O3(0001)/fcc(111)_sqrt13/Rh	-339.59	-345.02	-5.43	0.84
O-a-Al2O3(0001)/fcc(111)_sqrt3/Ru	-451.45	-441.62	9.83	3.53
O-a-Al2O3(0001)/fcc(111)_sqrt13/Ru	-390.18	-392.25	-2.06	0.41
O-a-SiO2(0001)/fcc(111)_sqrt3/Ag	-189.01	-190.41	-1.41	0.54
O-a-SiO2(0001)/fcc(111)_sqrt3/Au	-142.31	-146.90	-4.59	1.19
O-a-SiO2(0001)/fcc(111)_sqrt3/Cu	-267.85	-215.14	52.71	11.91
O-a-SiO2(0001)/fcc(111)_2x2/Cu	-238.28	-243.12	-4.84	1.73
O-a-SiO2(0001)/fcc(111)_sqrt3/Ir	-250.41	-224.36	26.06	5.22
O-a-SiO2(0001)/fcc(111)_sqrt3/Ni	-273.43	-224.61	48.82	14.35
O-a-SiO2(0001)/fcc(111)_2x2/Ni	-258.00	-248.07	9.93	1.09
O-a-SiO2(0001)/fcc(111)_sqrt3/Os	-277.51	-249.65	27.86	4.07
O-a-SiO2(0001)/fcc(111)_sqrt3/Pd	-203.19	-181.82	21.37	3.28
O-a-SiO2(0001)/fcc(111)_sqrt3/Pt	-201.32	-184.00	17.32	5.46
O-a-SiO2(0001)/fcc(111)_sqrt3/Rh	-244.23	-219.46	24.77	6.53
O-a-SiO2(0001)/fcc(111)_sqrt3/Ru	-293.16	-268.43	24.73	6.93
ZnO($11\bar{2}0$)/fcc(100)_2x2/Ag	-79.59	-85.92	-6.33	9.07
ZnO($11\bar{2}0$)/fcc(100)_2x2/Au	-79.26	-82.65	-3.39	9.75
ZnO($11\bar{2}0$)/fcc(100)_2x2/Cu	-118.22	-110.43	7.78	10.99
ZnO($11\bar{2}0$)/fcc(100)_2x2/Ir	-142.76	-140.96	1.80	4.25
ZnO($11\bar{2}0$)/fcc(100)_2x2/Ni	-184.49	-131.61	52.88	13.45
ZnO($11\bar{2}0$)/fcc(100)_2x2/Os	-166.92	-152.48	14.44	4.03
ZnO($11\bar{2}0$)/fcc(100)_2x2/Pd	-114.15	-115.21	-1.06	4.86
ZnO($11\bar{2}0$)/fcc(100)_2x2/Pt	-117.38	-118.03	-0.65	4.50
ZnO($11\bar{2}0$)/fcc(100)_2x2/Rh	-136.27	-134.02	2.25	5.55
ZnO($11\bar{2}0$)/fcc(100)_2x2/Ru	-172.83	-165.09	7.75	5.98
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Ag	-71.94	-91.34	-19.39	9.07
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Au	-55.25	-89.60	-34.35	9.75
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Cu	-106.29	-136.76	-30.47	11.00
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Ir	-94.15	-141.63	-47.49	4.24
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Ni	-111.98	-161.54	-49.56	13.46
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Os	-90.46	-121.79	-31.33	4.03
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Pd	-83.81	-133.31	-49.50	4.86
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Pt	-77.60	-137.33	-59.73	4.48
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Rh	-102.56	-148.25	-45.69	5.56
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Ru	-109.82	-147.29	-37.47	5.97

TiO2(110)/fcc(100)_sqrt5/Ag	-75.94	-84.61	-8.67	8.80
TiO2(110)/fcc(100)_sqrt5/Au	-62.31	-70.45	-8.15	9.49
TiO2(110)/fcc(100)_sqrt5/Ir	-116.99	-125.37	-8.38	14.09
TiO2(110)/fcc(100)_sqrt5/Os	-130.07	-128.57	1.50	16.47
TiO2(110)/fcc(100)_sqrt5/Pd	-98.31	-103.32	-5.01	5.69
TiO2(110)/fcc(100)_sqrt5/Pt	-88.63	-94.24	-5.61	7.81
TiO2(110)/fcc(100)_sqrt5/Rh	-119.96	-126.47	-6.51	8.85
TiO2(110)/fcc(100)_sqrt5/Ru	-144.88	-187.68	-42.80	9.24

Table S16. Interface energy, oxide energy, metal energy and surface area in Å^2 for all calculated metal/oxide structures of Table S15 with adjusting the metal to the oxid lattice constant. In the case of the hydroxylated oxide, the surface area of the strain-free oxide surface is used and the number of hydroxyl groups per supercell and the stability difference between hydroxylated and oxidized surfaces per supercell given. For the stoichiometric interfaces the surface area depending on the metal lattice constant is given.

Surface	$E_{Interface}$	E_{Oxide}	E_{Metal}	Area	N_{OH}	$\Delta\gamma^{ox}_{ox-lat}$
O-a-Al2O3(0001)/fcc(111)_sqrt3/Ag	-293.51	-272.58	-34.56	19.85	3	-414.39
O-a-Al2O3(0001)/fcc(111)_sqrt3/Au	-300.47	-272.58	-42.81	19.85	3	-414.39
O-a-Al2O3(0001)/fcc(111)_sqrt3/Cu	-304.23	-272.58	-44.27	19.85	3	-414.39
O-a-Al2O3(0001)/fcc(111)_sqrt3/Ir	-368.58	-272.58	-106.30	19.85	3	-414.39
O-a-Al2O3(0001)/fcc(111)_sqrt3/Ni	-322.51	-272.58	-60.44	19.85	3	-414.39
O-a-Al2O3(0001)/fcc(111)_sqrt3/Os	-394.46	-272.58	-130.92	19.85	3	-414.39
O-a-Al2O3(0001)/fcc(111)_sqrt13/Os	-1467.20	-1090.38	-421.02	79.38	12	-414.39
O-a-Al2O3(0001)/fcc(111)_sqrt3/Pd	-324.04	-272.58	-64.21	19.85	3	-414.39
O-a-Al2O3(0001)/fcc(111)_sqrt3/Pt	-336.78	-272.58	-76.34	19.85	3	-414.39
O-a-Al2O3(0001)/fcc(111)_sqrt3/Rh	-348.31	-272.58	-86.57	19.85	3	-414.39
O-a-Al2O3(0001)/fcc(111)_sqrt13/Rh	-1321.39	-1090.38	-277.51	79.38	12	-414.39
O-a-Al2O3(0001)/fcc(111)_sqrt3/Ru	-370.68	-272.58	-107.50	19.85	3	-414.39
O-a-Al2O3(0001)/fcc(111)_sqrt13/Ru	-1394.97	-1090.38	-347.07	79.38	12	-414.39
O-a-SiO2(0001)/fcc(111)_sqrt3/Ag	-247.62	-221.22	-34.94	21.33	2	-272.03
O-a-SiO2(0001)/fcc(111)_sqrt3/Au	-254.48	-221.22	-42.79	21.33	2	-272.03
O-a-SiO2(0001)/fcc(111)_sqrt3/Cu	-257.36	-221.22	-42.99	21.33	2	-272.03
O-a-SiO2(0001)/fcc(111)_2x2/Cu	-275.51	-221.22	-61.77	21.33	2	-272.03
O-a-SiO2(0001)/fcc(111)_sqrt3/Ir	-317.82	-221.22	-103.83	21.33	2	-272.03
O-a-SiO2(0001)/fcc(111)_sqrt3/Ni	-274.32	-221.22	-59.83	21.33	2	-272.03
O-a-SiO2(0001)/fcc(111)_2x2/Ni	-301.02	-221.22	-86.86	21.33	2	-272.03
O-a-SiO2(0001)/fcc(111)_sqrt3/Os	-342.84	-221.22	-128.27	21.33	2	-272.03
O-a-SiO2(0001)/fcc(111)_sqrt3/Pd	-276.32	-221.22	-63.34	21.33	2	-272.03
O-a-SiO2(0001)/fcc(111)_sqrt3/Pt	-288.03	-221.22	-75.08	21.33	2	-272.03
O-a-SiO2(0001)/fcc(111)_sqrt3/Rh	-298.46	-221.22	-84.60	21.33	2	-272.03
O-a-SiO2(0001)/fcc(111)_sqrt3/Ru	-320.11	-221.22	-105.20	21.33	2	-272.03
ZnO(11$\bar{2}$0)/fcc(100)_2x2/Ag	-105.78	-69.76	-33.38	33.19		
ZnO(11$\bar{2}$0)/fcc(100)_2x2/Au	-113.44	-69.76	-41.02	33.61		
ZnO(11$\bar{2}$0)/fcc(100)_2x2/Cu	-114.70	-69.76	-41.93	25.48		

ZnO($11\bar{2}0$)/fcc(100)_2x2/Ir	-173.81	-69.76	-99.84	29.49
ZnO($11\bar{2}0$)/fcc(100)_2x2/Ni	-132.29	-69.76	-57.05	24.09
ZnO($11\bar{2}0$)/fcc(100)_2x2/Os	-197.41	-69.76	-122.76	29.34
ZnO($11\bar{2}0$)/fcc(100)_2x2/Pd	-133.92	-69.76	-60.72	30.21
ZnO($11\bar{2}0$)/fcc(100)_2x2/Pt	-145.08	-69.76	-71.71	30.70
ZnO($11\bar{2}0$)/fcc(100)_2x2/Rh	-155.72	-69.76	-82.05	28.68
ZnO($11\bar{2}0$)/fcc(100)_2x2/Ru	-176.00	-69.76	-101.32	28.43
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Ag	-143.49	-105.72	-33.63	57.49
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Au	-150.78	-105.72	-41.84	58.22
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Cu	-152.09	-105.72	-41.68	44.13
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Ir	-212.39	-105.72	-101.86	51.07
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Ni	-168.68	-105.72	-57.54	41.72
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Os	-237.14	-105.72	-126.82	50.82
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Pd	-171.82	-105.72	-61.71	52.32
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Pt	-182.89	-105.72	-73.05	53.18
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Rh	-193.88	-105.72	-83.07	49.67
ZnO($10\bar{1}0$)/fcc(111)_2sqrt3x2/Ru	-215.04	-105.72	-103.92	49.25
TiO2(110)/fcc(100)_sqrt5/Ag	-469.62	-425.61	-40.86	41.49
TiO2(110)/fcc(100)_sqrt5/Au	-478.73	-425.61	-50.49	42.01
TiO2(110)/fcc(100)_sqrt5/Ir	-553.47	-425.61	-123.54	36.86
TiO2(110)/fcc(100)_sqrt5/Os	-583.47	-425.61	-153.09	36.68
TiO2(110)/fcc(100)_sqrt5/Pd	-504.84	-425.61	-75.52	37.76
TiO2(110)/fcc(100)_sqrt5/Pt	-518.07	-425.61	-89.06	38.38
TiO2(110)/fcc(100)_sqrt5/Rh	-531.39	-425.61	-101.48	35.85
TiO2(110)/fcc(100)_sqrt5/Ru	-556.89	-425.61	-126.13	35.54

S4 Cartesian coordinates of optimized structures

Oxide bulk structures

```
a-Al2O3 E_tot= -229.25706192 eV
Al  O
 1.0000000000000000
     4.7869999999999999    0.0000000000000000    0.0000000000000000
    -2.3934999999999991    4.1456636079161084    0.0000000000000000
     0.0000000000000008    0.0000000000000014   13.0449999999999999
  12  18
Cartesian
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  2.3934999394180401  1.3818877937350631  8.9413435174961027
 -0.0000000605819591  2.7637756630404309  0.2446768441302680
  0.0000000000000007  0.0000000149883486 11.1155101841627708
  2.3935000000000000  1.3818878842937175  2.4188435174961040
  0.0000000000000011  2.7637757535990874  6.7671768575286073
  0.0000000000000001 -0.0000000149883472  1.9294898091380599
  2.3935000000000004  1.3818878543170221  6.2778231558697311
  0.0000000000000013  2.7637757236223921 10.6261564758047253
  0.0000000605819603  0.0000000755703081  8.4519898158372300
  2.3935000605819612  1.3818879448756778 12.8003231424713917
  0.0000000605819607  2.7637758141810469  4.1036564825038946
  1.4679637852392722 -0.0000000605819595  3.2612500082891782
  3.8614637852392724  1.3818878087234101  7.6095833872161203
  1.4679637852392728  2.7637756780287797 11.9579166816550124
  0.7339818926196370  1.2712939270873349  9.7837499999999995
  3.1274818926196373  2.6531817963927020  1.0870833400325048
  0.7339818926196366  4.0350696656980727  5.4354166666666659
 -0.7339819532015952  1.2712939053998171  3.2612499917108217
  1.6595180467984052  2.6531817747051871  7.6095833250441576
 -0.7339819532015942  4.0350696440105569 11.9579166127838761
  3.3190362147607297  0.0000000605819609  9.7837499917108239
  0.9255362147607287  1.3818879298873297  1.0870832794505447
 -1.4679637852392711  2.7637757991926994  5.4354166516783193
  1.6595181073803655  2.8743696808287758  3.2612500000000000
  1.6595181073803649  0.1105939422180365  7.6095833266341648
 -0.7339818926196349  1.4924818115234062 11.9579166666666659
 -1.6595180467984030  2.8743697025162920  9.7837500082891751
  3.1274819532015954  0.1105939639055526  1.0870833416225139
  0.7339819532015964  1.4924818265117532  5.4354167205494548

TiO2 E_tot= -53.9004361 eV
Ti  O
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     4.6453148261374100   -0.0000018057035950   -0.0000000169370644
    -0.0000018050124767    4.6453148225021748   -0.0000000175509084
    -0.0000000105693610   -0.0000000114067044    2.9604196097496818
   2   4
Cartesian
 -0.0000018137512063  4.6453148108107518  2.9604195920755290
  2.3226565035402014  2.3226565022049930  1.4802097876476403
  1.4132728099332157  1.4132728068217433  2.9604195489329013
  3.2320402014768406  3.2320401992965158  0.0000000259139123
  0.9093737425534260  3.7359392643159488  1.4802097889107892
  3.7359392670545830  0.9093737411251737  1.4802097868722732

ZrO2 E_tot= -58.45890495 eV
 O Zr
 1.0000000000000000
     3.6077143316313793    0.0000000017398672    0.0000024391445645
```

```
     0.0000000027452017    3.6077149621394633    0.0000001827879476
     0.0000036130866827    0.0000002686925094    5.2392915673239981
   4   2
Cartesian
  3.6077143875210149  1.8038575898188713  1.0311041651985966
  1.8038585616449061  0.0000002236408008  4.2081913643820208
  0.0000041196821293  1.8038576862653737  3.6507472851687321
  1.8038588721066018  3.6077149775386848  1.5885455343849140
  3.6077167805560757  0.0000002753904709  5.2392935116724830
  1.8038602456300834  1.8038575992077992  2.6196475889265280

g-Al2O3 E_tot= -304.23341803 eV
 O Al
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     0.0000000000000000    8.3518925051664716    0.0000000000000000
     0.0000000000000000    0.0000000000000000    8.0348574396786834
  24  16
Cartesian
  4.9273756357848146  3.3912205363330967  7.2126489260957740
  3.3704343180175687  7.6661046463196820  4.9306106815463124
  1.9849985256043416  3.3922465423664545  6.8634780624934564
  0.7475257457147215  7.6589348371829438  5.1142592513057252
  0.6270812204574860  7.5668808119109769  0.8172617767221554
  2.1840625235238473  3.4905407920703997  3.0992309740796689
  3.5695115596019211  7.5681793290309489  1.1664037523379236
  4.8070467036385152  3.4835345897333378  2.9154487356820145
  0.6271197117217328  4.9553108461413036  0.8171846313585345
  2.1843055656233870  0.6803442598445294  3.0993087983151675
  3.5695827905894673  4.9545513690322771  1.1663033219798935
  4.8067642873160379  0.6877337709099717  2.9153264498660669
  4.9273382785488362  0.7796932595213686  7.2127530747595969
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  1.9849797806857461  0.7785696448889360  6.8632300946132050
  0.7474076890253052  4.8632259200559558  5.1141745469736222
  4.9021865269917475  6.2610956162476450  7.0393505466701045
  2.0177234115640728  6.2610519767213839  7.1434545487758099
  0.6525690994970849  2.0854352857038485  0.9904678229924032
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  3.4070632184772252  2.0856549109626621  5.1417451236794021
  0.7391983721283357  2.0855199633469259  5.0416382344276052
  2.1476192467159736  6.2611883152034196  2.8880058312546950
  4.8151341018710117  6.2612714531256186  2.9880825741920543
  2.0409937232202018  0.6271025807648632  4.9251767123034496
  0.6503790494514416  4.8315801277023516  6.9294301525055353
  3.5135072539220062  4.8030772736715202  3.1048001015807909
  4.9040807746614847  0.6557969025022298  1.1002232196823056
  3.5134671139276588  7.7194425804483169  3.1047479081959315
  4.9041845188651116  3.5149900566543661  1.1002824320877571
  2.0409637393257558  3.5434873191334870  4.9251015860278065
  0.6503318003821392  7.6907215676536156  6.9294878920836309
  2.1017942727302397  6.2609369556029968  1.0076245509835022
  4.8685327265134193  6.2613072733959809  1.0068229986262145
  3.4313410794198940  6.2610051590080120  5.9891563804498187
  3.4527660167819887  2.0858394055878611  7.0221661694142350
  0.6859915235436815  2.0853650581525431  7.0231988225629545
  2.1233067973783983  2.0854929554018948  2.0407296304193081
  4.8318990469532137  2.0856049662888472  4.0063260653273982
  0.7225518339024918  6.2610780210049040  4.0233225205900549

ZnO E_tot= -18.68048545 eV
Zn  O
 1.0000000000000000
```

```
     3.2740205373760505   -0.0000027862445941   -0.0000000509249036
    -1.6370126828356113    2.8353944377226830    0.0000000297714442
    -0.0000000892672285    0.0000000189371201    5.2827558095945903
   2   2
Cartesian
  1.6371719741028237  0.9451270117029533  5.2778152584100395
  0.0001628701181046  1.8902646728156365  2.6364373749211945
  1.6371722918445264  0.9451278358941848  3.2749663564126648
  0.0001631773428397  1.8902638243674288  0.6335884698116886

a-SiO2 E_tot= -72.05153822 eV
Si  O
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999992    4.2975558034858610    0.0000000000000000
     0.0000000000000003    0.0000000000000006    5.4538499999999992
   3   6
Cartesian
  2.3338921342252497  0.0000544474115309  3.6355943229264187
 -1.1669272721555870  2.0211505148605444  1.8183263302696746
  1.3145338210739885  2.2768680325859463  0.0000924523748453
  1.3834997374637763  1.1469305299685781  4.2836418197235675
  3.2770478159376317  0.6251245779289932  2.4658537384181254
  2.7829738397957939  2.5251265557203504  0.6472436621131357
  0.3014929910702306  1.7717823895851526  1.1703067450277957
 -1.0971323315682184  3.1504539720266078  2.9881814890186083
  0.7953993820825108  3.6727321126056243  4.8067047189907086

Oxidized and hydroxylated surfaces of the non stoichiometric surfaces

g-Al2O3 9OH_nm2 hydrox: E_tot= -712.14344878 eV, D3-zero damping= -
11.2283578 eV, D3-BJ damping= -16.7597843 eV
 O Al  O Al  O Al  H  O  H  O  H  O  H
 1.0000000000000000
     8.3518925051664716    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.0348574396786834    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.0605986182420502
  18  12  24  16  12   8   1   1   1   1   1   1   3
Selective dynamics
Cartesian
  3.3912205363330972  7.2126489260957740 10.9423958550990683   F   F   F
  7.6661046463196820  4.9306106815463115  9.3854545373318228   F   F   F
  3.3922465423664545  6.8634780624934573  8.0000187449185951   F   F   F
  3.4905407920703997  3.0992309740796689  8.1990827428381010   F   F   F
  7.5681793290309489  1.1664037523379236  9.5845317789161744   F   F   F
  3.4835345897333378  2.9154487356820149 10.8220669229527680   F   F   F
  0.6803442598445294  3.0993087983151675  8.1993257849376402   F   F   F
  4.9545513690322771  1.1663033219798935  9.5846030099037201   F   F   F
  0.6877337709099717  2.9153264498660669 10.8217845066302907   F   F   F
  0.7796932595213686  7.2127530747595978 10.9423584978630899   F   F   F
  4.8557882337421594  4.9306965981488604  9.3853700880230981   F   F   F
  0.7785696448889361  6.8632300946132050  8.0000000000000000   F   F   F
  6.2610956162476450  7.0393505466701054 10.9172067463060021   F   F   F
  6.2610519767213839  7.1434545487758099  8.0327436308783255   F   F   F
  2.0857684421935652  0.8863033110849516  9.5519775531218265   F   F   F
  2.0856549109626621  5.1417451236794021  9.4220834377914784   F   F   F
  6.2611883152034196  2.8880058312546955  8.1626394660302282   F   F   F
  6.2612714531256195  2.9880825741920547 10.8301543211852653   F   F   F
  0.6271025807648632  4.9251767123034496  8.0560139425344559   F   F   F
  4.8030772736715202  3.1048001015807913  9.5285274732362595   F   F   F
  0.6557969025022298  1.1002232196823056 10.9191009939757393   F   F   F
  7.7194425804483151  3.1047479081959319  9.5284873332419124   F   F   F
  3.5149900566543661  1.1002824320877571 10.9192047381793653   F   F   F
```

3.5434873191334866	4.9251015860278065	8.0559839586400095	F	F	F
6.2609369556029968	1.0076245509835022	8.1168144920444938	F	F	F
6.2613072733959809	1.0068229986262147	10.8835529458276739	F	F	F
6.2610051590080129	5.9891563804498196	9.4463612987341481	F	F	F
2.0858394055878611	7.0221661694142350	9.4677862360962415	F	F	F
2.0854929554018948	2.0407296304193077	8.1383270166926529	F	F	F
2.0856049662888472	4.0063260653273982	10.8469192662674665	F	F	F
3.3876665108043120	7.1676344540947001	16.5362776010521060	T	T	T
7.6710995274276410	4.9202261791655406	14.9538900961669157	T	T	T
3.3922465423664545	6.8634780624934573	13.5580397357678457	F	F	F
7.6589348371829438	5.1142592513057252	12.3205669558782276	F	F	F
7.5668808119109761	0.8172617767221555	12.2001224306209899	F	F	F
3.4905407920703997	3.0992309740796689	13.7571037336873516	F	F	F
7.5492812701461309	1.1586230943336029	15.1068093250220379	T	T	T
3.4794806786782337	2.8930105965854889	16.3808043297761046	T	T	T
4.9553108461413045	0.8171846313585345	12.2001609218852369	F	F	F
0.6803442598445294	3.0993087983151675	13.7573467757868890	F	F	F
4.9660806676880540	1.1546433292215865	15.1665885307410022	T	T	T
0.6805615807818299	2.8766471702259899	16.3766401092527119	T	T	T
0.8215681550075784	7.1453198005942573	16.4633373418079785	T	T	T
4.8540320246970188	4.9261200548714106	14.9595188902890524	T	T	T
0.7785696448889361	6.8632300946132050	13.5580209908492506	F	F	F
4.8632259200559558	5.1141745469736231	12.3204488991888095	F	F	F
6.2305015956805168	6.9895164847677194	16.5007201202256297	T	T	T
6.2610519767213839	7.1434545487758099	13.5907646217275762	F	F	F
2.0854352857038485	0.9904678229924032	12.2256103096605884	F	F	F
2.0947072907948980	0.8699020037718828	15.0999491127948424	T	T	T
2.0909895585778879	5.1174092666373943	14.9557436997498954	T	T	T
2.0855199633469259	5.0416382344276061	12.3122395822918396	F	F	F
6.2611883152034196	2.8880058312546955	13.7206604568794788	F	F	F
6.2638880542283228	2.9949832875281626	16.3893535529468899	T	T	T
0.6271025807648632	4.9251767123034496	13.6140349333837065	F	F	F
4.8315801277023516	6.9294301525055353	12.2234202596149455	F	F	F
4.8138610108665221	3.0935820262253553	15.0895291874066366	T	T	T
0.6248987121244187	1.0292969887879861	16.4228172934101266	T	T	T
7.7097518003941214	3.0868574911867541	15.0803310273295725	T	T	T
3.4981080217028291	1.0609850434545764	16.4254025291536081	T	T	T
3.5434873191334866	4.9251015860278065	13.6140049494892601	F	F	F
7.6907215676536156	6.9294878920836309	12.2233730105456431	F	F	F
6.2609369556029968	1.0076245509835022	13.6748354828937444	F	F	F
6.2851196968671790	1.0285968604897218	16.5217372776344611	T	T	T
6.2677385306826734	5.9869414297359294	15.0017490905630115	T	T	T
2.0773908603607136	6.9881061937573028	15.0430005120203862	T	T	T
2.0853650581525431	7.0231988225629554	12.2590327337071869	F	F	F
2.0854929554018948	2.0407296304193077	13.6963480075419035	F	F	F
2.0692463606079583	3.9512961885229765	16.3264565173701612	T	T	T
6.2610780210049048	4.0233225205900549	12.2955930440659955	F	F	F
3.4833875664611700	6.7490791683509608	19.0651829707455249	T	T	T
7.6533010943550233	5.0677552147227356	17.9924469916253003	T	T	T
7.6601525563725028	0.7774906768140832	17.6605565449668092	T	T	T
3.4130653304458427	2.8678332256328538	19.3671548623939529	T	T	T
4.8480785746817414	0.8635586846921055	17.7487163499655729	T	T	T
0.5282951002534771	3.1246848047551179	19.4731164148029166	T	T	T
0.7146820940539994	6.7778857508727510	19.0828983064063884	T	T	T
4.8376519574330361	4.9726733398248752	18.0025691256726574	T	T	T
6.2081647731469216	6.9660464304743055	19.0611423145631456	T	T	T
2.0577432652056080	0.9620088928472531	17.8026519319440375	T	T	T
2.0941710990337339	4.9425714738424089	17.8279755680559333	T	T	T
6.2636583713624923	2.8807701946891009	19.2670055712671271	T	T	T
0.7174416828543865	4.9384509903765226	19.0810721108980097	T	T	T
4.8665638270629730	6.8334346020620202	17.7591295976783101	T	T	T
3.4333700587624896	4.6757466199482325	19.0451818446833592	T	T	T
7.6557380927216219	6.9698526890722858	17.8919511385266752	T	T	T

```
  4.9013821013876706  1.8193815402265587 19.3117140326158570   T   T   T
  2.0408050639828987  7.0785398311202545 17.8762702038485095   T   T   T
  1.8607621417758591  1.9082257077031581 19.3376736911296874   T   T   T
  6.2978843439455554  3.9739973266497901 17.9014414028442488   T   T   T
 -0.4462263534330551  2.8080901370250380 19.4386557536545155   T   T   T
  1.8685934062223890  0.8507351914837626 20.7098655535668783   T   T   T
  1.3736369013156120  0.0165649594513307 20.5744191362928817   T   T   T
  4.6815500474685194  0.6097773991346875 20.5775006693283089   T   T   T
  3.9122198612500032  0.7648663062364445 21.1642867359473961   T   T   T
  2.1638466516650445  4.9497229957066642 20.4026417501280086   T   T   T
  2.1090906324293486  4.2538578603659891 21.0785559633399977   T   T   T
  3.7185577783530586  7.3662764525866873 19.8228686096403841   T   T   T
  6.0643617487473005  7.5078777990240626 19.8585589075390274   T   T   T

g-Al2O3 9OH_nm2 ox: E_tot= -676.94517396 eV, D3-zero damping= -10.7865814
eV, D3-BJ damping= -16.2736959 eV
 O Al  O Al  O Al  O
 1.0000000000000000
     8.3518925051664716    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.0348574396786834    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.7098655535668783
  18  12  24  16  12   8   3
Selective dynamics
Cartesian
  3.3912205363330972  7.2126489260957740 10.9423958550990683   F   F   F
  7.6661046463196820  4.9306106815463115  9.3854545373318228   F   F   F
  3.3922465423664545  6.8634780624934573  8.0000187449185951   F   F   F
  3.4905407920703997  3.0992309740796689  8.1990827428381010   F   F   F
  7.5681793290309489  1.1664037523379236  9.5845317789161744   F   F   F
  3.4835345897333378  2.9154487356820149 10.8220669229527680   F   F   F
  0.6803442598445294  3.0993087983151675  8.1993257849376402   F   F   F
  4.9545513690322771  1.1663033219798935  9.5846030099037201   F   F   F
  0.6877337709099717  2.9153264498660669 10.8217845066302907   F   F   F
  0.7796932595213686  7.2127530747595978 10.9423584978630899   F   F   F
  4.8557882337421594  4.9306965981488604  9.3853700880230981   F   F   F
  0.7785696448889361  6.8632300946132050  8.0000000000000000   F   F   F
  6.2610956162476450  7.0393505466701054 10.9172067463060021   F   F   F
  6.2610519767213839  7.1434545487758099  8.0327436308783255   F   F   F
  2.0857684421935652  0.8863033110849516  9.5519775531218265   F   F   F
  2.0856549109626621  5.1417451236794021  9.4220834377914784   F   F   F
  6.2611883152034196  2.8880058312546955  8.1626394660302282   F   F   F
  6.2612714531256195  2.9880825741920547 10.8301543211852653   F   F   F
  0.6271025807648632  4.9251767123034496  8.0560139425344559   F   F   F
  4.8030772736715202  3.1048001015807913  9.5285274732362595   F   F   F
  0.6557969025022298  1.1002232196823056 10.9191009939757393   F   F   F
  7.7194425804483151  3.1047479081959319  9.5284873332419124   F   F   F
  3.5149900566543661  1.1002824320877571 10.9192047381793653   F   F   F
  3.5434873191334866  4.9251015860278065  8.0559839586400095   F   F   F
  6.2609369556029968  1.0076245509835022  8.1168144920444938   F   F   F
  6.2613072733959809  1.0068229986262147 10.8835529458276739   F   F   F
  6.2610051590080129  5.9891563804498196  9.4463612987341481   F   F   F
  2.0858394055878611  7.0221661694142350  9.4677862360962415   F   F   F
  2.0854929554018948  2.0407296304193077  8.1383270166926529   F   F   F
  2.0856049662888472  4.0063260653273982 10.8469192662674665   F   F   F
  3.3862227179420250  7.2032246247344229 16.5197041462100387   T   T   T
  7.6654560798554865  4.9178573200589053 14.9420347811308307   T   T   T
  3.3922465423664545  6.8634780624934573 13.5580397357678457   F   F   F
  7.6589348371829438  5.1142592513057252 12.3205669558782276   F   F   F
  7.5668808119109761  0.8172617767221555 12.2001224306209899   F   F   F
  3.4905407920703997  3.0992309740796689 13.7571037336873516   F   F   F
  7.5521681121232991  1.1503797676388585 15.0869809960646553   T   T   T
  3.4673728986209515  2.8787666219948176 16.3478539029830756   T   T   T
  4.9553108461413045  0.8171846313585345 12.2001609218852369   F   F   F
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  0.6803442598445294  3.0993087983151675 13.7573467757868890   F   F   F
  4.9651173525498367  1.1560467964369583 15.1395228291058537   T   T   T
  0.6670401613891807  2.8637114962957959 16.3753749143843343   T   T   T
  0.8480180307763623  7.1744826653301343 16.4890757220206119   T   T   T
  4.8574475100930750  4.9240800016239294 14.9352505697868523   T   T   T
  0.7785696448889361  6.8632300946132050 13.5580209908492506   F   F   F
  4.8632259200559558  5.1141745469736231 12.3204488991888095   F   F   F
  6.2175574801093907  7.0283910004608838 16.4953227330449721   T   T   T
  6.2610519767213839  7.1434545487758099 13.5907646217275762   F   F   F
  2.0854352857038485  0.9904678229924032 12.2256103096605884   F   F   F
  2.0904213206631668  0.8789711824343474 15.0914804153746207   T   T   T
  2.0888329518340956  5.1139181099962734 14.9321993848135950   T   T   T
  2.0855199633469259  5.0416382344276061 12.3122395822918396   F   F   F
  6.2611883152034196  2.8880058312546955 13.7206604568794788   F   F   F
  6.2653431846224992  2.9807262739013112 16.3844614421744126   T   T   T
  0.6271025807648632  4.9251767123034496 13.6140349333837065   F   F   F
  4.8315801277023516  6.9294301525055353 12.2234202596149455   F   F   F
  4.8201162531624142  3.0974112226641757 15.1081057508186642   T   T   T
  0.6287199159231225  1.0216199886523136 16.4441044661016420   T   T   T
  7.6994415230267350  3.0791891033048908 15.0949363876309341   T   T   T
  3.5089962092614662  1.0490754620182081 16.4126648418456682   T   T   T
  3.5434873191334866  4.9251015860278065 13.6140049494892601   F   F   F
  7.6907215676536156  6.9294878920836309 12.2233730105456431   F   F   F
  6.2609369556029968  1.0076245509835022 13.6748354828937444   F   F   F
  6.2779270277981150  0.9768370319361643 16.4972537105915933   T   T   T
  6.2628095395920553  5.9954433704898902 15.0447396812083483   T   T   T
  2.0869163937398767  6.9888686196603800 15.0959869166046996   T   T   T
  2.0853650581525431  7.0231988225629554 12.2590327337071869   F   F   F
  2.0854929554018948  2.0407296304193077 13.6963480075419035   F   F   F
  2.0570962735553668  3.9333674929495630 16.3010100312647594   T   T   T
  6.2610780210049048  4.0233225205900549 12.2955930440659955   F   F   F
  3.4327066758357296  6.5924195569666439 19.0536524166415866   T   T   T
  7.6281932311493881  5.0783932809233274 18.0328888738199353   T   T   T
  7.6475470081288988  0.8006977339231888 17.6507989328469179   T   T   T
  3.6640301203713168  2.9654479943491778 19.2217598564191761   T   T   T
  4.8432590640596924  0.8678626054452915 17.7433199709694875   T   T   T
  1.0479667542829341  3.3135016205110244 19.8337864519229221   T   T   T
  0.7081173594333657  6.8117623971720320 19.0883833247327672   T   T   T
  4.9224098130338918  4.9705941814566650 17.9403851080398802   T   T   T
  6.1726171630300728  7.1284468597394506 19.1005630414107479   T   T   T
  2.0716826131148571  0.9962285605601885 17.8659887165883831   T   T   T
  2.0434662852359775  4.8915209734633649 17.7725492302500072   T   T   T
  6.3977034094979555  2.8125455146137299 19.2901959874399935   T   T   T
  0.7025823210902098  5.0183648991773175 19.0390839843138657   T   T   T
  4.8505097618163449  6.8357823374589275 17.8847186974332928   T   T   T
  3.4580434084059308  4.7559259156343430 18.9516850857605661   T   T   T
  7.6029191268325418  7.0211238527272313 17.9859965103985004   T   T   T
  5.0418935983230639  1.7848062120904340 19.2917417394972937   T   T   T
  2.0829173983998341  7.0882890925995508 17.9449519384405178   T   T   T
  2.2099044199441562  1.9927612841624331 19.3400831484183726   T   T   T
  6.3357384958400633  3.9122112714694564 17.9466438579620409   T   T   T
  2.8624617156989265  0.9008069676601356 20.7129272978605883   T   T   T
  4.2396662268877821  0.8343004150624829 20.7073416371794785   T   T   T
  1.9150082144153115  4.5133079909768092 20.3352606363110091   T   T   T

a-Al2O3 hydrox: E_tot= -545.13523491 eV, D3-zero damping= -9.1439347 eV,
D3-BJ damping= -13.4144726 eV
Al  O Al  O  H Al  O Al  O  H
 1.0000000000000000
     4.7869999999999999    0.0000000000000000    0.0000000000000000
    -4.7869999999999981    8.2913272158322169    0.0000000000000000
     0.0000000000000000    0.0000000000000000   30.8056962042704043
  10  18   2   3   6  10  18   2   3   6
```

Cartesian

2.3978093518165315	4.1331928565748610	12.3904880956250825
2.3961624445627128	1.3747738137051564	16.7369115340058023
0.0047529618286859	-0.0040596231370274	18.9215183011896748
2.3983556581126875	1.3692404238172025	10.0981621619845257
0.0038790758264654	2.7550933723471567	14.5558176081972093
2.4296607094760598	4.1468420221847744	9.7770407814429863
2.3984671769614851	1.3726150950077132	14.0667325606806717
0.0005427879062921	2.7598255248858665	18.4131839506451165
0.0028235077117884	-0.0078299894724100	16.2482293166841600
0.0095514294640811	2.7521530301493629	11.8832454254944135
-0.9042552805790299	4.1368931466198875	11.0346096527810058
3.8658661636232332	1.3737536774048884	15.4018749885858206
1.4843449654518259	2.7575784586316838	19.7705809469777272
0.7358829508709213	1.2667744783951669	17.5824554533984099
3.1313383902392986	2.6995924030460574	8.8713457027060407
0.7399392072894795	4.0247600468782938	13.2236208271297055
4.0472141923409257	1.2713638587580356	11.0360089902158407
1.6631461921439357	2.6452091002579370	15.4012224027742786
-0.7284051910856320	4.0384307962237580	19.7649165696281557
3.3228449531753110	-0.0077971840509329	17.5795525862508342
0.9134975545852998	1.3161156076237994	8.8482913410074886
-1.4610503278268585	2.7558204276656033	13.2248476262868504
1.6706210349036881	2.8555725020772140	11.0400140952309602
1.6629163360037511	0.1025621564813484	15.4025647498638634
-0.7450236348602455	1.4770820289772268	19.7680414664939335
-1.6568212540701293	2.8689389039269066	17.5799451346540572
3.1984930325992309	0.0454135380734732	8.9144439680591674
0.7384563305165011	1.4811324637362473	13.2214476990774266
2.3926922151528500	1.3789302291884085	20.7067686066151886
0.0299238724346110	2.7475858481958078	21.0276466243205107
3.1935308093287542	2.7014030969179279	21.8923441921731232
0.9070181280338684	1.4320071617168246	21.9554995170137808
3.1239739015570342	0.0486896884512896	21.9352754995055292
0.3916593065133077	0.5931919222257833	21.9776159756204414
3.1331779537652551	2.3886643511008798	22.8056858756989769
2.6414302987631046	0.1838880673157877	22.7671625213843214
0.3982606082924250	2.1551744583137262	8.8258806917291324
2.6532590882307359	2.5662285543435384	8.0367817090608700
3.1301670408280629	0.3527387986152693	7.9998968428571429
0.0043093518165326	8.2788564644909695	12.3904880956250825
0.0026624445627138	5.5204374216212644	16.7369115340058023
-2.3887470381713132	4.1416039847790804	18.9215183011896748
0.0048556581126882	5.5149040317333107	10.0981621619845257
-2.3896209241735336	6.9007569802632656	14.5558176081972093
0.0361607094760608	8.2925056301008837	9.7770407814429863
0.0049671769614859	5.5182787029238209	14.0667325606806717
-2.3929572120937070	6.9054891328019750	18.4131839506451165
-2.3906764922882107	4.1378336184436977	16.2482293166841600
-2.3839485705359178	6.8978166380654722	11.8832454254944135
-3.2977552805790293	8.2825567545359959	11.0346096384952919
1.4723661636232339	5.5194172853209968	15.4018749885858206
-0.9091550345481730	6.9032420665477927	19.7705809612634411
-1.6576170491290778	5.4124380863112753	17.5824554533984099
0.7378384045250139	6.8452560109621654	8.8713456884203268
-1.6535607927105198	8.1704236547944014	13.2236208271297055
1.6537141923409266	5.4170274809598586	11.0360089902158407
-0.7303538078560635	6.7908727081740450	15.4012224027742786
-3.1219051910856312	8.1840943898541507	19.7649165696281557
0.9293449531753118	4.1378664238651757	17.5795525862508342
-1.4800024454146994	5.4617792155399085	8.8482913410074886
-3.8545503278268574	6.9014840355817118	13.2248476262868504
-0.7228789650963111	7.0012360957076085	11.0400140952309602

```
 -0.7305836639962480  4.2482257643974570 15.4025647498638634
 -3.1385236348602445  5.6227456368933355 19.7680414664939335
 -4.0503212540701279  7.0146025118430142 17.5799451346540572
  0.8049930325992318  4.1910771459895813  8.9144439680591674
 -1.6550436694834980  5.6267960716523557 13.2214476990774266
 -0.0008077848471488  5.5245938371045167 20.7067686066151886
 -2.3635761275653882  6.8932494561119162 21.0276466243205107
  0.8000308093287554  6.8470667048340363 21.8923442064588372
 -1.4864818719661306  5.5776707696329337 21.9554995312994947
  0.7304739015570352  4.1943532963673986 21.9352754995055292
 -2.0018406934866912  4.7388555301418913 21.9776159756204414
  0.7396779537652562  6.5343279590169887 22.8056858756989769
  0.2479302987631057  4.3295516752318957 22.7671625213843214
 -1.9952393917075741  6.3008380662298347  8.8258806917291324
  0.2597590882307367  6.7118921622596464  8.0367817090608700
  0.7366670408280637  4.4984024065313779  7.9998968428571429

a-SiO2 ox: E_tot= -256.87781904 eV, D3-zero damping= -2.750185 eV, D3-BJ
damping= -3.9511541 eV
Si  O Si  O Si  O Si  O  H
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999992    4.2975558034858610    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.8592805318753562
   3   6   3   6   3   6   1   4   2
Cartesian
  2.3902371008396130 -0.1531311866489961 14.5075531659320802
  3.7818532714170661  1.8958012291901465 12.6719811686341135
  1.2820764822838739  2.2626884074103422 10.8618932135077131
  1.4430773077653118  0.9875156970902372 15.1739567231680539
  3.2821929519643538  0.4857687792310579 13.3083909238091564
  2.7014509470337766  2.4998176612629783 11.6155063354731567
  0.2333281471107488  1.6025324390257740 11.9225298315108521
 -1.0201578782582408  2.9692263295434582 13.8869239123805315
  0.8823720662400936  3.5331376152847587 15.6647501698996159
  2.4036474875615199 -0.1496464196452469 19.9656078207725436
  3.8616914991197482  1.8756203811522367 18.1484158670936750
  1.3825484340468555  2.1354639229511947 16.3257344762296697
  1.4581610215718337  1.0005858947490254 20.6165620686793112
  3.3455237016441841  0.4745885259751033 18.7935182279932036
  2.8490301050473246  2.3846018199446597 16.9815349172379797
  0.3707127483896924  1.6416460813155007 17.5041340889857402
 -1.0320467771305357  2.9984243597402549 19.3289611018138636
  0.8677379893207270  3.5266408707636878 21.1401266174514646
  2.1435941581356870  0.1013110902213809 25.2734388735425881
  3.8852775915679012  1.8916591903343929 23.6022819715538290
  1.4005188730575182  2.1341438816451084 21.7821929634197886
  3.3466544243402283  0.4932564106175897 24.2497585351416447
  2.8758607079792675  2.3831713193537420 22.4185813735375810
  0.3950899125381960  1.6177491404581885 22.9630659422758860
 -1.0128637266683727  3.0380662660239648 24.7504259609628541
  1.2048284014009594  1.3127315166781166 25.8674772165152511
 -0.2780198108182513  4.7755225394785175 26.8640182731826691
  2.4044104618858193  0.0586402953354395  9.0337331301633910
  1.5118340992618056  1.3174277998236756  9.5596907347412330
  3.5899589978910997  0.6737150319011295  8.0596230144163528
 -1.1811383768447015  3.4356228077799362  8.2650344824879287
  0.6571311618110726  3.6591125973487224 10.3189199002153380
  4.4279488468363946  0.1591539484667818  8.0159991343204702
 -1.1114642417612921  2.4575545495160398  8.1203409523825094

g-Al2O3 6OH_nm2 hydrox: E_tot= -695.78448805 eV, D3-zero damping= -
10.9642822 eV, D3-BJ damping= -16.4654671 eV
```

```
 O Al  O Al  O Al  H  O  H  O  H
 1.0000000000000000
     8.3518925051664716    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.0348574396786834    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.4682785053458538
  18  12  24  16  12   8   1   1   1   1   2
Selective dynamics
Cartesian
  3.3912205363330972  7.2126489260957740 10.9423958550990683   F   F   F
  7.6661046463196820  4.9306106815463115  9.3854545373318228   F   F   F
  3.3922465423664545  6.8634780624934573  8.0000187449185951   F   F   F
  3.4905407920703997  3.0992309740796689  8.1990827428381010   F   F   F
  7.5681793290309489  1.1664037523379236  9.5845317789161744   F   F   F
  3.4835345897333378  2.9154487356820149 10.8220669229527680   F   F   F
  0.6803442598445294  3.0993087983151675  8.1993257849376402   F   F   F
  4.9545513690322771  1.1663033219798935  9.5846030099037201   F   F   F
  0.6877337709099717  2.9153264498660669 10.8217845066302907   F   F   F
  0.7796932595213686  7.2127530747595978 10.9423584978630899   F   F   F
  4.8557882337421594  4.9306965981488604  9.3853700880230981   F   F   F
  0.7785696448889361  6.8632300946132050  8.0000000000000000   F   F   F
  6.2610956162476450  7.0393505466701054 10.9172067463060021   F   F   F
  6.2610519767213839  7.1434545487758099  8.0327436308783255   F   F   F
  2.0857684421935652  0.8863033110849516  9.5519775531218265   F   F   F
  2.0856549109626621  5.1417451236794021  9.4220834377914784   F   F   F
  6.2611883152034196  2.8880058312546955  8.1626394660302282   F   F   F
  6.2612714531256195  2.9880825741920547 10.8301543211852653   F   F   F
  0.6271025807648632  4.9251767123034496  8.0560139425344559   F   F   F
  4.8030772736715202  3.1048001015807913  9.5285274732362595   F   F   F
  0.6557969025022298  1.1002232196823056 10.9191009939757393   F   F   F
  7.7194425804483151  3.1047479081959319  9.5284873332419124   F   F   F
  3.5149900566543661  1.1002824320877571 10.9192047381793653   F   F   F
  3.5434873191334866  4.9251015860278065  8.0559839586400095   F   F   F
  6.2609369556029968  1.0076245509835022  8.1168144920444938   F   F   F
  6.2613072733959809  1.0068229986262147 10.8835529458276739   F   F   F
  6.2610051590080129  5.9891563804498196  9.4463612987341481   F   F   F
  2.0858394055878611  7.0221661694142350  9.4677862360962415   F   F   F
  2.0854929554018948  2.0407296304193077  8.1383270166926529   F   F   F
  2.0856049662888472  4.0063260653273982 10.8469192662674665   F   F   F
  3.3712436776871755  7.2204117557566745 16.5822247434652894   T   T   T
  7.6684126844820328  4.9122674634670771 14.9513857228809748   T   T   T
  3.3922465423664545  6.8634780624934573 13.5580397357678457   F   F   F
  7.6589348371829438  5.1142592513057252 12.3205669558782276   F   F   F
  7.5668808119109761  0.8172617767221555 12.2001224306209899   F   F   F
  3.4905407920703997  3.0992309740796689 13.7571037336873516   F   F   F
  7.5796927127131459  1.1345209830549048 15.1099850239231124   T   T   T
  3.5000189621437729  2.8975095002698517 16.3837337597322055   T   T   T
  4.9553108461413045  0.8171846313585345 12.2001609218852369   F   F   F
  0.6803442598445294  3.0993087983151675 13.7573467757868890   F   F   F
  4.9464489661982549  1.1410154073306236 15.1098052751856073   T   T   T
  0.6566967106456678  2.8952494918975495 16.3941380084631376   T   T   T
  0.8247431357176718  7.2146405722793299 16.5904673551644386   T   T   T
  4.8521152035495785  4.9152088605003170 14.9543418664593872   T   T   T
  0.7785696448889361  6.8632300946132050 13.5580209908492506   F   F   F
  4.8632259200559558  5.1141745469736231 12.3204488991888095   F   F   F
  6.2460636411211548  7.0123040541617030 16.4687757459715662   T   T   T
  6.2610519767213839  7.1434545487758099 13.5907646217275762   F   F   F
  2.0854352857038485  0.9904678229924032 12.2256103096605884   F   F   F
  2.0845707936356850  0.8940830593108842 15.1414073352184584   T   T   T
  2.0838120232333983  5.1333450797223836 14.9729123209460226   T   T   T
  2.0855199633469259  5.0416382344276061 12.3122395822918396   F   F   F
  6.2611883152034196  2.8880058312546955 13.7206604568794788   F   F   F
  6.2641135971265509  2.9354070705923263 16.3421796581568231   T   T   T
  0.6271025807648632  4.9251767123034496 13.6140349333837065   F   F   F
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```
  4.8315801277023516  6.9294301525055353 12.2234202596149455   F   F   F
  4.8127689294065705  3.0808005784545713 15.0712763493467978   T   T   T
  0.6539843097601757  1.0743255474944662 16.5199707797179869   T   T   T
  7.7097648438367994  3.0747336625416866 15.0649187022794422   T   T   T
  3.5048365672687352  1.0816296258324092 16.4907658352660960   T   T   T
  3.5434873191334866  4.9251015860278065 13.6140049494892601   F   F   F
  7.6907215676536156  6.9294878920836309 12.2233730105456431   F   F   F
  6.2609369556029968  1.0076245509835022 13.6748354828937444   F   F   F
  6.2671395612595537  0.9321900865447412 16.3878711713554850   T   T   T
  6.2617484281045623  5.9771933258717640 14.9967138804738589   T   T   T
  2.0818295447828632  7.0107085842973378 15.0987152509504128   T   T   T
  2.0853650581525431  7.0231988225629554 12.2590327337071869   F   F   F
  2.0854929554018948  2.0407296304193077 13.6963480075419035   F   F   F
  2.0791689662274035  3.9307086055853331 16.3071472757430165   T   T   T
  6.2610780210049048  4.0233225205900549 12.2955930440659955   F   F   F
  3.4955415727065025  6.6021372307104089 19.0975095468084000   T   T   T
  7.6068015109447789  5.0599539839036014 17.8805214885345158   T   T   T
  7.5810734755024693  0.8155875897977031 17.7235640784497832   T   T   T
  3.4221197989233341  3.2761514590945477 19.7164543373452688   T   T   T
  4.9180118342375136  0.8763832472915654 17.6977029622373969   T   T   T
  0.6464428586618737  3.2736796328416125 19.6397012152773947   T   T   T
  0.7278583733146695  6.6489423953522655 19.1401130451415256   T   T   T
  4.9780456735979994  4.9757026467364982 17.9069925332296478   T   T   T
  6.2514529259980183  7.2282943904673251 19.0810564089866261   T   T   T
  2.0739761777968901  1.0702148673751763 17.9243990380458094   T   T   T
  2.1036566603584701  4.8524649660565036 17.8240032861612789   T   T   T
  6.5801800950103750  2.7493432968620000 19.2069518387544811   T   T   T
  0.6517296643564928  4.8513321804107381 18.8906516681357886   T   T   T
  4.8835139513526995  6.8528770060236024 17.8486772751693614   T   T   T
  3.5680839154674939  4.7916115143616889 18.9005481900527030   T   T   T
  7.6565127713172512  6.9292182226050079 17.8929157800587930   T   T   T
  6.0803566358723415  0.9829088605327648 19.1013781616971698   T   T   T
  2.1075340392703010  7.1685915584324693 18.0473686252822141   T   T   T
  2.0422851750206399  2.1599925776846396 19.5117523955478944   T   T   T
  6.3256289017409895  3.8863187808353916 17.8283970670006653   T   T   T
 -0.7476263645025191  2.8853702283666776 19.4855031621689392   T   T   T
  2.2532108715896619  0.9341415396432343 20.7414540130002685   T   T   T
  1.7616691454008693  0.0963415684357442 20.6961874260566496   T   T   T
  4.9195327495864811  1.2819693580880527 20.5391017661132587   T   T   T
  4.5019799283744248  2.2066733994216605 20.3828372258067212   T   T   T
  4.0945057921888770  0.7301457197413157 20.6954030230365262   T   T   T

a-Al2O3 ox: E_tot= -507.23402158 eV, D3-zero damping= -8.5963859 eV, D3-BJ
damping= -12.8416286 eV
Al  O Al  O  H Al  O Al  O  H
 1.0000000000000000
     4.7869999999999999    0.0000000000000000    0.0000000000000000
    -4.7869999999999981    8.2913272158322169    0.0000000000000000
     0.0000000000000000    0.0000000000000000   30.7324665057619946
  10  18   2   3   3  10  18   2   3   3
Cartesian
  2.3996503662667124  4.1015599804958764 12.4097781351084127
  2.3974885188506518  1.3420512559975510 16.7425520372382302
 -0.0331454897164587 -0.0931745021686950 18.9193077507283611
  2.4011181050910224  1.3405978209860026 10.1143800807832740
  0.0021972956949417  2.7213394741748793 14.5769239947765286
  2.4329975025923027  4.1185806151640323  9.7968727622434191
  2.3993122394284079  1.3351216057451887 14.0788451970922601
  0.0254779150739093  2.7180388990483331 18.4695607278070248
  0.0091734984985535 -0.0378963676348209 16.2626825926707248
  0.0118635062131519  2.7205072322387069 11.9013716820847151
 -0.9015779474243520  4.1079217711446665 11.0621818231912616
  3.8633838579735511  1.3339158072267492 15.4195018010748051
```

1.4946672852970000	2.7124057125232661	19.6528319177376360
0.7343917791971977	1.2034029627194318	17.5915554884853158
3.1408435420867362	2.6732535574935565	8.9008448967810310
0.7423792129449253	3.9894107424699072	13.2513364804368177
4.0481083464668393	1.2389482763605792	11.0621403979424340
1.6583398047116154	2.6099908109238767	15.4336910156263158
-0.7971089534512189	3.9636873384185711	19.8779707767242648
3.3009950418625711	-0.0452480695234021	17.6132525436854337
0.9185086135018898	1.2896444374181089	8.8793016325859568
-1.4612668599598373	2.7234853333304532	13.2515730524085704
1.6745010615557026	2.8252229309029975	11.0656673977032920
1.6650400913490397	0.0619064631665992	15.4226573306531165
-0.6922128393037974	1.4447347708082201	19.7684033376434947
-1.6288930873771488	2.8296571368887462	17.5890519226550630
3.2032402070603343	0.0198898815238545	8.9372848303533186
0.7387706871305716	1.4476445344787272	13.2469679909869278
2.3579233336754855	1.3437869792223678	20.3143981370622733
-0.4270722741826821	2.7082102045836964	21.3041720752031019
2.8419712032492854	1.7968854512074219	21.9861337012152234
0.9849267932886985	2.9444164530705219	22.3281254506486171
3.1691481183856185	0.2882052504436939	21.9553165480006278
0.4061444062089050	2.1299442133606399	8.8499404800361638
2.7035411449255711	2.5466520025359349	8.0433288924840252
3.1290966301463246	0.3061170877669830	8.0160765957236695
0.0067407993097571	8.2452624760516944	12.4077106338270280
-0.0006451667846281	5.4793434897052364	16.7578737133709907
-2.3943908154478826	4.1235801377676591	18.9543059021056983
0.0079626235011880	5.4861862427816082	10.1147202528902547
-2.3874129681164957	6.8613714152131964	14.5768897534534201
0.0389374925075066	8.2642267186713063	9.7954457319758337
0.0085049624318029	5.4820862933729373	14.0881127414282830
-2.3875427579608579	6.8369145208715452	18.4648877326674565
-2.3892821120631753	4.0969736752108723	16.2790134654523122
-2.3810806447431179	6.8662857558205346	11.9018816386922790
-3.2950709726867227	8.2528249646852121	11.0613810161133319
1.4752495052375065	5.4831429997302124	15.4336136458019890
-0.9742145136069119	6.8501885467741808	19.7411928218032600
-1.6664736472568720	5.3589366016631788	17.6236065505662580
0.7471117151790319	6.8188462293682628	8.8997976158811980
-1.6501481613835749	8.1328195371094480	13.2482491796462014
1.6554428252050624	5.3848730339963424	11.0634290276565110
-0.7304568457803876	6.7551042529581302	15.4419328229358115
-3.1890588371283246	8.1219689405127227	19.8031732637301090
0.9174535052121088	4.1266258965909293	17.6266202104392669
-1.4752614303855978	5.4349123891775033	8.8790653769228491
-3.8544985318313825	6.8671081997532362	13.2530331967744530
-0.7185388901089866	6.9704388137390501	11.0649792997475949
-0.7302052235133811	4.2166069061737810	15.4289363091790790
-3.0934399370308161	5.5544815260907106	19.9555176113877799
-4.0461166549640559	6.9520378278848698	17.6308823386556774
0.8098077544007851	4.1652363147843658	8.9384687047878248
-1.6531788072803617	5.5935815278513772	13.2512070571909710
0.0389734197000201	5.4362745446066825	20.7919904134407894
-2.3300512066698218	7.0335093410054395	21.1766821857060457
0.4614979770798379	6.8978379098426448	21.8783444868403052
-0.9279590486291089	6.2805053537623703	22.2271378588098081
0.0546592115115398	4.1877766997057408	22.2599122716866873
-1.9874206405993391	6.2753408382734701	8.8496807145677128
0.3086164666306329	6.6908503162495823	8.0430902752067706
0.7366273763634140	4.4524271714670771	8.0174135882219080

g-Al2O3 6OH_nm2 ox: E_tot= -672.68550886 eV, D3-zero damping= -10.7284121 eV, D3-BJ damping= -16.1928718 eV

```
 O Al  O Al  O Al  O
 1.0000000000000000
     8.3518925051664716    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.0348574396786834    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.7414540130002685
  18  12  24  16  12   8   2
Selective dynamics
Cartesian
  3.3912205363330972  7.2126489260957740 10.9423958550990683   F   F   F
  7.6661046463196820  4.9306106815463115  9.3854545373318228   F   F   F
  3.3922465423664545  6.8634780624934573  8.0000187449185951   F   F   F
  3.4905407920703997  3.0992309740796689  8.1990827428381010   F   F   F
  7.5681793290309489  1.1664037523379236  9.5845317789161744   F   F   F
  3.4835345897333378  2.9154487356820149 10.8220669229527680   F   F   F
  0.6803442598445294  3.0993087983151675  8.1993257849376402   F   F   F
  4.9545513690322771  1.1663033219798935  9.5846030099037201   F   F   F
  0.6877337709099717  2.9153264498660669 10.8217845066302907   F   F   F
  0.7796932595213686  7.2127530747595978 10.9423584978630899   F   F   F
  4.8557882337421594  4.9306965981488604  9.3853700880230981   F   F   F
  0.7785696448889361  6.8632300946132050  8.0000000000000000   F   F   F
  6.2610956162476450  7.0393505466701054 10.9172067463060021   F   F   F
  6.2610519767213839  7.1434545487758099  8.0327436308783255   F   F   F
  2.0857684421935652  0.8863033110849516  9.5519775531218265   F   F   F
  2.0856549109626621  5.1417451236794021  9.4220834377914784   F   F   F
  6.2611883152034196  2.8880058312546955  8.1626394660302282   F   F   F
  6.2612714531256195  2.9880825741920547 10.8301543211852653   F   F   F
  0.6271025807648632  4.9251767123034496  8.0560139425344559   F   F   F
  4.8030772736715202  3.1048001015807913  9.5285274732362595   F   F   F
  0.6557969025022298  1.1002232196823056 10.9191009939757393   F   F   F
  7.7194425804483151  3.1047479081959319  9.5284873332419124   F   F   F
  3.5149900566543661  1.1002824320877571 10.9192047381793653   F   F   F
  3.5434873191334866  4.9251015860278065  8.0559839586400095   F   F   F
  6.2609369556029968  1.0076245509835022  8.1168144920444938   F   F   F
  6.2613072733959809  1.0068229986262147 10.8835529458276739   F   F   F
  6.2610051590080129  5.9891563804498196  9.4463612987341481   F   F   F
  2.0858394055878611  7.0221661694142350  9.4677862360962415   F   F   F
  2.0854929554018948  2.0407296304193077  8.1383270166926529   F   F   F
  2.0856049662888472  4.0063260653273982 10.8469192662674665   F   F   F
  3.3564760512219194  7.2038194097725263 16.5213435609762804   T   T   T
  7.6710901858114910  4.9139252265975015 14.9417354140106990   T   T   T
  3.3922465423664545  6.8634780624934573 13.5580397357678457   F   F   F
  7.6589348371829438  5.1142592513057252 12.3205669558782276   F   F   F
  7.5668808119109761  0.8172617767221555 12.2001224306209899   F   F   F
  3.4905407920703997  3.0992309740796689 13.7571037336873516   F   F   F
  7.5740657501328039  1.1454005708723309 15.0977396386162006   T   T   T
  3.4823467000182817  2.8835542879975362 16.3737290067998131   T   T   T
  4.9553108461413045  0.8171846313585345 12.2001609218852369   F   F   F
  0.6803442598445294  3.0993087983151675 13.7573467757868890   F   F   F
  4.9510228893073442  1.1450262347267595 15.0961195368117291   T   T   T
  0.6684976097380555  2.8889211783338573 16.3940258130653156   T   T   T
  0.8131389899709753  7.2143576960463109 16.5760516878888140   T   T   T
  4.8558691186232306  4.9161913243677695 14.9310507552360239   T   T   T
  0.7785696448889361  6.8632300946132050 13.5580209908492506   F   F   F
  4.8632259200559558  5.1141745469736231 12.3204488991888095   F   F   F
  6.2608759022677560  7.0262483555163389 16.4692453888554269   T   T   T
  6.2610519767213839  7.1434545487758099 13.5907646217275762   F   F   F
  2.0854352857038485  0.9904678229924032 12.2256103096605884   F   F   F
  2.0744346750889306  0.8910026203310590 15.1221910943498337   T   T   T
  2.0802941912560802  5.1281052420764262 14.9467267798717049   T   T   T
  2.0855199633469259  5.0416382344276061 12.3122395822918396   F   F   F
  6.2611883152034196  2.8880058312546955 13.7206604568794788   F   F   F
  6.2606448854356431  2.9449148820510604 16.3634461308474641   T   T   T
  0.6271025807648632  4.9251767123034496 13.6140349333837065   F   F   F
```

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  4.8315801277023516  6.9294301525055353 12.2234202596149455   F   F   F
  4.8206192198618822  3.0876769759142020 15.0962617680279099   T   T   T
  0.6355633422764535  1.0680180881907082 16.5486389741534197   T   T   T
  7.7060129936358939  3.0781897534566443 15.0947661885768269   T   T   T
  3.4993171325300856  1.0534973470718425 16.4379332648686507   T   T   T
  3.5434873191334866  4.9251015860278065 13.6140049494892601   F   F   F
  7.6907215676536156  6.9294878920836309 12.2233730105456431   F   F   F
  6.2609369556029968  1.0076245509835022 13.6748354828937444   F   F   F
  6.2761862907019088  0.9468581521646072 16.4051306364151159   T   T   T
  6.2646157270805372  5.9766314201764352 15.0269974105027817   T   T   T
  2.0662503245963011  7.0077409435957296 15.1147140174631929   T   T   T
  2.0853650581525431  7.0231988225629554 12.2590327337071869   F   F   F
  2.0854929554018948  2.0407296304193077 13.6963480075419035   F   F   F
  2.0754823462680547  3.9402841699057740 16.3020980253734002   T   T   T
  6.2610780210049048  4.0233225205900549 12.2955930440659955   F   F   F
  3.4911289480844219  6.6494960460741046 19.0488308602702361   T   T   T
  7.5720311333161598  5.0140495459345011 17.9603936018158628   T   T   T
  7.5746868530287790  0.8197028796866676 17.7207266156774921   T   T   T
  3.5738626613102831  3.3709598038768291 19.6047282494991428   T   T   T
  4.8732934796685869  0.8409326433180183 17.6607616449630207   T   T   T
  0.9277839843716016  3.2119239290941173 19.6649420802089132   T   T   T
  0.7163170017582665  6.6035684297018529 19.1374624754292100   T   T   T
  4.9798636508206862  5.0339932050033873 17.8075218923106533   T   T   T
  6.2078299793927352  7.2793967480526129 19.1009043088697403   T   T   T
  2.1000231848077431  1.0288812120132527 17.9293793417115630   T   T   T
  2.0873181678632209  4.9158269274013957 17.7776270349313208   T   T   T
  6.2955696110129926  2.7211824303243377 19.2838745188481688   T   T   T
  0.6493138645952240  4.7667886951751983 18.9246798045365345   T   T   T
  4.8768567998363741  6.8867201810538266 17.8090810639009938   T   T   T
  3.5891792977546575  4.8792993067988748 18.8310191974914680   T   T   T
  7.6351133822649979  6.9168214488973909 17.9702731996532066   T   T   T
  5.9332300511938945  1.0312827875451882 19.1323050762680076   T   T   T
  2.0740935947492583  7.0984147500292556 18.0177090293883744   T   T   T
  2.3289095488261742  2.1922659257290653 19.3579235481108505   T   T   T
  6.2686795149658341  3.8404759065294165 17.9387812847151302   T   T   T
  3.2571936035052285  1.0124371955499187 20.6149298255468345   T   T   T
  4.5705064420210206  0.8432374758130557 20.6015742903191921   T   T   T

a-SiO2 hydrox: E_tot= -269.43867193 eV, D3-zero damping= -2.8528963 eV, D3-
BJ damping= -4.0637742 eV
Si  O Si  O Si  O  H Si  O  H
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999992    4.2975558034858610    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.5309895818938912
   3   6   3   6   3   6   2   1   4   2
Cartesian
  2.3393089079106626 -0.0570035903163405 14.4482687820911782
  3.7376673657891160  1.9890285049161778 12.6139941207877886
  1.2407661228445748  2.3513483831445745 10.8055579038054450
  1.3863009315746868  1.0792240313592891 15.1132329705170640
  3.2273973900103434  0.5812328550587156 13.2434661945145997
  2.6651655695514287  2.5928871438410077 11.5465796472943456
  0.1929691597552639  1.6957819374121701 11.8685786694399820
 -1.0688965459385309  3.0629837282343324 13.8266037957091790
  0.8419220087844922  3.6311689136813512 15.5949827098776677
  2.3394992297603827 -0.0052184424116291 19.8949839308260898
  3.8232196098224009  2.0003848917991047 18.0835479178142116
  1.3423625682891120  2.2350359360280692 16.2609403673335784
  1.4133909902032873  1.1711503645525099 20.5203954659589485
  3.3201309758366935  0.6039528244264689 18.7456010014946557
  2.8188205269964999  2.4751058921772184 16.8935328250319721
  0.3379810846741988  1.7623151220897080 17.4517129532095829
```

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 -1.0951056447259719  3.1544323688170497 19.2331636097849703
  0.7516768997370622  3.6568606273847815 21.0968477948503406
  2.3631820280430511 -0.1891450018535521 25.3677180033643062
  3.7293225415783580  1.9016461920584751 23.5367044033852757
  1.2641174070224530  2.2513539547108929 21.7285764186747308
  3.1004020947280329  0.5104264351003340 24.0886657604022112
  2.6863855872470155  2.5491585723646701 22.4639261814189375
  0.1955362841809530  1.6553303718697341 22.8046212668473203
 -1.0173528011343322  2.8572546456472758 24.8361813910800500
  1.2672938938833367  0.7294036304615948 26.1521640773786004
  1.0692742338142942  3.4863070313549271 26.3383816510675501
  1.3305987712539020  1.7109353537327958 26.2789761747234536
  1.9104405452792270  3.9968337269145890 26.3690275085079406
  2.3630195174455912  0.1480518200299802  8.9763739736325583
  1.4640046722926321  1.4027184419411651  9.5015414851286106
  3.5522777245940409  0.7679145640570211  8.0067553484822529
 -1.2121548704842362  3.5244113181367229  8.1923699625142596
  0.6147973487333335  3.7461536210308619 10.2585238060773047
  4.3925736802032285  0.2558265107327263  7.9755948026741041
 -1.1499839868443311  2.5419203457439967  8.0713576883187148
```

Oxygen coverage dependent adsorption structures

```
O_fcc111-3x3x4-freeze-2/Au E_tot= -132.73978931 eV
Au  O
 1.0000000000000000
     8.6962551314100036    0.0000000000000000    0.0000000000000000
     4.3481275657050018    7.5311778615918419    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.1617043952762849
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.4493758552350002  0.8367975401768712 10.3668208605571532   F   F   F
  0.0175227832789610  1.6632727849142273 12.7647008946544407   T   T   T
 -0.1419354605160691 -0.0820955934157954 15.2322403317758326   T   T   T
  1.4493758552350002  2.5103926205306140  8.0000000000000000   F   F   F
  2.8987517104700005  3.3471901607074850 10.3668208605571532   F   F   F
  1.4493245126385217  4.1550718217981588 12.7229802990871068   T   T   T
  1.4492400151137395  2.6739517456312454 15.2322152235369757   T   T   T
  2.8987517104700005  5.0207852410612279  8.0000000000000000   F   F   F
  4.3481275657050018  5.8575827812380989 10.3668208605571532   F   F   F
  2.9235844294815223  6.7084413154070495 12.7228279501048576   T   T   T
  2.8942988154982419  5.0232625905463832 15.1052251348004472   T   T   T
  2.8987517104700005  0.0000000000000000  8.0000000000000000   F   F   F
  4.3481275657050018  0.8367975401768712 10.3668208605571532   F   F   F
  2.8812411748523532  1.6633541223660555 12.7646209627142735   T   T   T
  3.0405141007006535 -0.0822472171124263 15.2322143039597275   T   T   T
  4.3481275657050018  2.5103926205306140  8.0000000000000000   F   F   F
  5.7975034209400009  3.3471901607074850 10.3668208605571532   F   F   F
  4.3388895960230149  4.1891309352088930 12.6947080389539479   T   T   T
  4.3705466709185989  2.5229616397369994 15.0885554078528923   T   T   T
  5.7975034209400009  5.0207852410612279  8.0000000000000000   F   F   F
  7.2468792761750009  5.8575827812380989 10.3668208605571532   F   F   F
  5.7974875201482758  6.7143571888490801 12.7647431692996296   T   T   T
  5.7973536443893474  4.9942725924604074 15.0886713778051007   T   T   T
  5.7975034209400009  0.0000000000000000  8.0000000000000000   F   F   F
  7.2468792761750009  0.8367975401768712 10.3668208605571532   F   F   F
  5.7974892247943943  1.6625726357590209 12.6947534147165868   T   T   T
  5.7973414508171226 -0.0053511681229984 15.1052261434306416   T   T   T
  7.2468792761750009  2.5103926205306140  8.0000000000000000   F   F   F
  8.6962551314100001  3.3471901607074850 10.3668208605571532   F   F   F
```

```
  7.2560333098870693  4.1891134659960017 12.6946903876678743   T   T   T
  7.2241340018924829  2.5230641989140565 15.0885932175560296   T   T   T
  8.6962551314100036  5.0207852410612279  8.0000000000000000   F   F   F
 10.1456309866450027  5.8575827812380989 10.3668208605571532   F   F   F
  8.6713721026433213  6.7084481017414976 12.7228781677141747   T   T   T
  8.7005178322931975  5.0232647779263155 15.1051702067935203   T   T   T
  1.4492182356895020  0.8365320796336323 16.3260561361050591   T   T   T

O_fcc111-3x3x4-freeze-2/Ag E_tot= -110.14314209 eV
Ag  O
 1.0000000000000000
     8.6415811558500017    0.0000000000000000    0.0000000000000000
     4.3207905779250009    7.4838288098309915    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.1103911782774496
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.4402635259750003  0.8315365344256657 10.3519404891869975   F   F   F
  0.0061355599293990  1.6592325640089420 12.7001838332012831   T   T   T
 -0.0795202818565783 -0.0463718148899160 15.0968774065096927   T   T   T
  1.4402635259750003  2.4946096032769973  8.0000000000000000   F   F   F
  2.8805270519500006  3.3261461377026627 10.3519404891869975   F   F   F
  1.4401743348930365  4.1379816754603249 12.6824967579766668   T   T   T
  1.4400178165115263  2.5860506613111403 15.0967060570176059   T   T   T
  2.8805270519500006  4.9892192065539946  8.0000000000000000   F   F   F
  4.3207905779250009  5.8207557409796600 10.3519404891869975   F   F   F
  2.8973397928019375  6.6617512994102386 12.6824732660051929   T   T   T
  2.8784106701274701  4.9899259900371211 15.0227110967965221   T   T   T
  2.8805270519500006  0.0000000000000000  8.0000000000000000   F   F   F
  4.3207905779250009  0.8315365344256657 10.3519404891869975   F   F   F
  2.8741811035923539  1.6592150309955886 12.7001907676444237   T   T   T
  2.9601295042210110 -0.0466987802774420 15.0968091057618246   T   T   T
  4.3207905779250009  2.4946096032769973  8.0000000000000000   F   F   F
  5.7610541039000012  3.3261461377026627 10.3519404891869975   F   F   F
  4.3154605194311895  4.1603935803866374 12.6759145125922643   T   T   T
  4.3354390054866689  2.5026204432347732 15.0340111755501056   T   T   T
  5.7610541039000012  4.9892192065539946  8.0000000000000000   F   F   F
  7.2013176298750006  5.8207557409796600 10.3519404891869975   F   F   F
  5.7609686038381627  6.6591665817667636 12.7002594912655375   T   T   T
  5.7609178106705157  4.9714372551711312 15.0341122315795914   T   T   T
  5.7610541039000012  0.0000000000000000  8.0000000000000000   F   F   F
  7.2013176298750006  0.8315365344256657 10.3519404891869975   F   F   F
  5.7609415696473683  1.6566980150523716 12.6759702234983482   T   T   T
  5.7610275494427983 -0.0029526291508440 15.0226457986082593   T   T   T
  7.2013176298750006  2.4946096032769973  8.0000000000000000   F   F   F
  8.6415811558500000  3.3261461377026627 10.3519404891869975   F   F   F
  7.2064706995886478  4.1604121902198905 12.6759015932617416   T   T   T
  7.1863188406134961  2.5027001646197378 15.0340720653066775   T   T   T
  8.6415811558500017  4.9892192065539946  8.0000000000000000   F   F   F
 10.0818446818250020  5.8207557409796600 10.3519404891869975   F   F   F
  8.6246691784606533  6.6617703502591636 12.6825121783654904   T   T   T
  8.6434278581399866  4.9898115358431898 15.0228162746974334   T   T   T
  1.4405646026926353  0.8311698121426533 16.3199929975635882   T   T   T

O_fcc111-3x3x4-freeze-2/Cu E_tot= -145.46965009 eV
Cu  O
 1.0000000000000000
     7.5713089101900026    0.0000000000000000    0.0000000000000000
     3.7856544550950013    6.5569458561240124    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.1059075747554417
  36   1
Selective dynamics
```

```
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.2618848183650002  0.7285495395693347 10.0606492794392555   F   F   F
  0.0073469649918051  1.4527039049442012 12.1237329267332594   T   T   T
 -0.0559633970283024 -0.0325938033519014 14.2587784619728293   T   T   T
  1.2618848183650002  2.1856486187080040  8.0000000000000000   F   F   F
  2.5237696367300004  2.9141981582773386 10.0606492794392555   F   F   F
  1.2616733792939623  3.6226983397818393 12.1107827651544877   T   T   T
  1.2620334339882151  2.2492171830720551 14.2590181510791503   T   T   T
  2.5237696367300004  4.3712972374160080  8.0000000000000000   F   F   F
  3.7856544550950013  5.0998467769853431 10.0606492794392555   F   F   F
  2.5405403026653710  5.8379098527242705 12.1107536989720170   T   T   T
  2.5199822189512111  4.3727846806222583 14.1414237446539719   T   T   T
  2.5237696367300004  0.0000000000000000  8.0000000000000000   F   F   F
  3.7856544550950013  0.7285495395693347 10.0606492794392555   F   F   F
  2.5162658639741471  1.4526022608848190 12.1237939741159089   T   T   T
  2.5791396126180799 -0.0320722213593215 14.2589974382926901   T   T   T
  3.7856544550950013  2.1856486187080040  8.0000000000000000   F   F   F
  5.0475392734600009  2.9141981582773386 10.0606492794392555   F   F   F
  3.7795966600875066  3.6458564824039286 12.0967244951923707   T   T   T
  3.8094091607494529  2.1990972292966267 14.1532651330863217   T   T   T
  5.0475392734600009  4.3712972374160080  8.0000000000000000   F   F   F
  6.3094240918250009  5.0998467769853431 10.0606492794392555   F   F   F
  5.0475558540309740  5.8367068772725963 12.1237369118403215   T   T   T
  5.0479992165922525  4.3441465907705856 14.1531751932611325   T   T   T
  5.0475392734600009  0.0000000000000000  8.0000000000000000   F   F   F
  6.3094240918250009  0.7285495395693347 10.0606492794392555   F   F   F
  5.0473403224702853  1.4500511488081043 12.0967268258333487   T   T   T
  5.0471657621217734 -0.0044165945337212 14.1414253146458382   T   T   T
  6.3094240918250009  2.1856486187080040  8.0000000000000000   F   F   F
  7.5713089101900009  2.9141981582773386 10.0606492794392555   F   F   F
  6.3153712161689093  3.6460110753161539 12.0965564008637863   T   T   T
  6.2863676480336590  2.1992122002879615 14.1531794055018239   T   T   T
  7.5713089101900026  4.3712972374160080  8.0000000000000000   F   F   F
  8.8331937285550026  5.0998467769853431 10.0606492794392555   F   F   F
  7.5539908551752850  5.8379839881547619 12.1107877731777602   T   T   T
  7.5752011618074997  4.3732624489872025 14.1415846915944368   T   T   T
  1.2611335770495828  0.7278208309113737 15.3949067534743040   T   T   T

O_fcc111-3x3x4-freeze-2/Pt E_tot= -235.20038141 eV
Pt  O
 1.0000000000000000
     8.3113600962600014    0.0000000000000000    0.0000000000000000
     4.1556800481300007    7.1978489833614363    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.8004685009017756
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3852266827100002  0.7997609981512707 10.2620657004851434   F   F   F
  0.0043394903721959  1.5967132548377512 12.5175529086470121   T   T   T
 -0.0894556668756911 -0.0520565317935882 14.8602475106622762   T   T   T
  1.3852266827100002  2.3992829944538121  8.0000000000000000   F   F   F
  2.7704533654200003  3.1990439926050827 10.2620657004851434   F   F   F
  1.3851729721833139  3.9854344546559246 12.5351163734462503   T   T   T
  1.3851374513990868  2.5019704276235259 14.8600344365400172   T   T   T
  2.7704533654200003  4.7985659889076242  8.0000000000000000   F   F   F
  4.1556800481300007  5.5983269870588952 10.2620657004851434   F   F   F
  2.7818402390655255  6.4045008667891992 12.5351920035331386   T   T   T
  2.7710928257600269  4.7977567729787056 14.8223147016033945   T   T   T
  2.7704533654200003  0.0000000000000000  8.0000000000000000   F   F   F
  4.1556800481300007  0.7997609981512707 10.2620657004851434   F   F   F
  2.7660279153370304  1.5967588761874825 12.5175610820287204   T   T   T
```

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  2.8597890363671463 -0.0520695999995651 14.8602510213295851   T   T   T
  4.1556800481300007  2.3992829944538121  8.0000000000000000   F   F   F
  5.5409067308400006  3.1990439926050827 10.2620657004851434   F   F   F
  4.1533039590645711  3.9998311545808876 12.5011903015079930   T   T   T
  4.1726316542886543  2.4088529690752933 14.7886882954381935   T   T   T
  5.5409067308400006  4.7985659889076242  8.0000000000000000   F   F   F
  6.9261334135499997  5.5983269870588952 10.2620657004851434   F   F   F
  5.5408685130755568  6.4031470466281508 12.5175418595510308   T   T   T
  5.5408562055454276  4.7787714949671978 14.7884097441007469   T   T   T
  5.5409067308400006  0.0000000000000000  8.0000000000000000   F   F   F
  6.9261334135499997  0.7997609981512707 10.2620657004851434   F   F   F
  5.5408597066663230  1.5966389475320721 12.5011839199833350   T   T   T
  5.5408393200307016  0.0006747392732317 14.8222558973412362   T   T   T
  6.9261334135499997  2.3992829944538121  8.0000000000000000   F   F   F
  8.3113600962599996  3.1990439926050827 10.2620657004851434   F   F   F
  6.9283937398142275  3.9998805667210298 12.5011753546235269   T   T   T
  6.9090591130550667  2.4088839458553273 14.7886309032389924   T   T   T
  8.3113600962600014  4.7985659889076242  8.0000000000000000   F   F   F
  9.6965867789700013  5.5983269870588952 10.2620657004851434   F   F   F
  8.2999339705186497  6.4045095730894452 12.5351806576660145   T   T   T
  8.3106284496765159  4.7978142451290182 14.8223615021257054   T   T   T
  1.3851839165706907  0.7992858398725983 15.9880994657500555   T   T   T

O_fcc111-3x3x4-freeze-2/Pd E_tot= -199.28307611 eV
Pd  O
 1.0000000000000000
     8.2439436957000023    0.0000000000000000    0.0000000000000000
     4.1219718478500011    7.1394646678447691    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.7371961239475979
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3739906159500004  0.7932738519827520 10.2437172802999097   F   F   F
  0.0020482782684997  1.5850464002716282 12.4807620885653812   T   T   T
 -0.0532657305364014 -0.0311420016146748 14.8024258460001832   T   T   T
  1.3739906159500004  2.3798215559482561  8.0000000000000000   F   F   F
  2.7479812319000008  3.1730954079310081 10.2437172802999097   F   F   F
  1.3739206892770530  3.9577070438592843 12.5133934325735030   T   T   T
  1.3742471040147426  2.4409630711755539 14.8021942318413462   T   T   T
  2.7479812319000008  4.7596431118965121  8.0000000000000000   F   F   F
  4.1219718478500011  5.5529169638792641 10.2437172802999097   F   F   F
  2.7557155012761263  6.3505236892879049 12.5120630301806433   T   T   T
  2.7476343904160792  4.7601563596518606 14.7707306457865002   T   T   T
  2.7479812319000008  0.0000000000000000  8.0000000000000000   F   F   F
  4.1219718478500011  0.7932738519827520 10.2437172802999097   F   F   F
  2.7466748361345314  1.5856212708680948 12.4792180690851833   T   T   T
  2.8013230808852536 -0.0310405002715404 14.8020265284269534   T   T   T
  4.1219718478500011  2.3798215559482561  8.0000000000000000   F   F   F
  5.4959624638000015  3.1730954079310081 10.2437172802999097   F   F   F
  4.1188387439617395  3.9670935669423386 12.4731297103468357   T   T   T
  4.1397011535169517  2.3897151256129496 14.7339262126782078   T   T   T
  5.4959624638000015  4.7596431118965121  8.0000000000000000   F   F   F
  6.8699530797500010  5.5529169638792641 10.2437172802999097   F   F   F
  5.4958086287443351  6.3485777199765074 12.4807053120077871   T   T   T
  5.4956448939474116  4.7396013424053951 14.7346125640789136   T   T   T
  5.4959624638000015  0.0000000000000000  8.0000000000000000   F   F   F
  6.8699530797500010  0.7932738519827520 10.2437172802999097   F   F   F
  5.4951657094890463  1.5833627630501488 12.4731492036454128   T   T   T
  5.4964371666418632 -0.0011184161160538 14.7707979218474232   T   T   T
  6.8699530797500010  2.3798215559482561  8.0000000000000000   F   F   F
  8.2439436957000005  3.1730954079310081 10.2437172802999097   F   F   F
  6.8727656541027038  3.9678362703840060 12.4749234292415814   T   T   T
```

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  6.8528617196009245  2.3887739314472807 14.7346721325734347   T   T   T
  8.2439436957000023  4.7596431118965121  8.0000000000000000   F   F   F
  9.6179343116500018  5.5529169638792641 10.2437172802999097   F   F   F
  8.2364235068392926  6.3501699070956024 12.5133073747322374   T   T   T
  8.2444641307359738  4.7596138104009054 14.7715291898405710   T   T   T
  1.3739257543025389  0.7929524093476633 15.9171853733059265   T   T   T

O_fcc111-3x3x4-freeze-2/Ni E_tot= -202.88836157 eV
Ni  O
 1.0000000000000000
     7.3615742453100017    0.0000000000000000    0.0000000000000000
     3.6807871226550009    6.3753103082837166    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.9090651051721714
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.2269290408850002  0.7083678120315240 10.0035667338470748   F   F   F
  0.0046007123166842  1.4140128033626733 12.0154395598863957   T   T   T
 -0.0325044170953468 -0.0188324930258767 14.1135296008374365   T   T   T
  1.2269290408850002  2.1251034360945722  8.0000000000000000   F   F   F
  2.4538580817700004  2.8334712481260960 10.0035667338470748   F   F   F
  1.2268691840069073  3.5343789403385273 12.0203862774944987   T   T   T
  1.2269195139458653  2.1624459064148178 14.1134235864227424   T   T   T
  2.4538580817700004  4.2502068721891444  8.0000000000000000   F   F   F
  3.6807871226550009  4.9585746842206682 10.0035667338470748   F   F   F
  2.4602267066071555  5.6702792918946781 12.0203266222563325   T   T   T
  2.4513469231483693  4.2513826238575936 14.0002387650552276   T   T   T
  2.4538580817700004  0.0000000000000000  8.0000000000000000   F   F   F
  3.6807871226550009  0.7083678120315240 10.0035667338470748   F   F   F
  2.4492048336271850  1.4139495779990423 12.0154006870648917   T   T   T
  2.4862863526759038 -0.0189287225781243 14.1135898434097573   T   T   T
  3.6807871226550009  2.1251034360945722  8.0000000000000000   F   F   F
  4.9077161635400008  2.8334712481260960 10.0035667338470748   F   F   F
  3.6773422469233621  3.5433784059141749 11.9982996260998327   T   T   T
  3.7111711640201452  2.1422702805970588 14.0002350660176020   T   T   T
  4.9077161635400008  4.2502068721891444  8.0000000000000000   F   F   F
  6.1346452044250004  4.9585746842206682 10.0035667338470748   F   F   F
  4.9076913825605759  5.6719171693060035 12.0155827362488079   T   T   T
  4.9077099416174557  4.2148053364669771 14.0000490222374463   T   T   T
  4.9077161635400008  0.0000000000000000  8.0000000000000000   F   F   F
  6.1346452044250004  0.7083678120315240 10.0035667338470748   F   F   F
  4.9076703052329096  1.4123453902700485 11.9984247879233621   T   T   T
  4.9076933861304246 -0.0033723847750209 14.0002608411673375   T   T   T
  6.1346452044250004  2.1251034360945722  8.0000000000000000   F   F   F
  7.3615742453099999  2.8334712481260960 10.0035667338470748   F   F   F
  6.1379550179895013  3.5433744669095990 11.9982501690754813   T   T   T
  6.1041416168117584  2.1422795612663537 14.0002607169530222   T   T   T
  7.3615742453100017  4.2502068721891444  8.0000000000000000   F   F   F
  8.5885032861950013  4.9585746842206682 10.0035667338470748   F   F   F
  7.3551240168933907  5.6702677610340961 12.0203398025908399   T   T   T
  7.3640181620805514  4.2513898556382550 14.0002757932188970   T   T   T
  1.2268690661470854  0.7083104893152741 15.2275026713037693   T   T   T

O_fcc111-3x3x4-freeze-2/Ir E_tot= -327.67817904 eV
Ir  O
 1.0000000000000000
     8.1451896436500029    0.0000000000000000    0.0000000000000000
     4.0725948218250014    7.0539411500428191    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6445123918711744
  36   1
Selective dynamics
Cartesian
```

```
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3575316072750003  0.7837712388936464 10.2168398316827176   F   F   F
  0.0029673537350673  1.5657833833827584 12.3959429524809188   T   T   T
 -0.0348012112967394 -0.0202580414503682 14.6535600852226526   T   T   T
  1.3575316072750003  2.3513137166809397  8.0000000000000000   F   F   F
  2.7150632145500007  3.1350849555745857 10.2168398316827176   F   F   F
  1.3575165966426217  3.9094748513277500 12.4164573103076137   T   T   T
  1.3577052957376128  2.3911237607093110 14.6539489244427781   T   T   T
  2.7150632145500007  4.7026274333618794  8.0000000000000000   F   F   F
  4.0725948218250014  5.4863986722555254 10.2168398316827176   F   F   F
  2.7229953673035419  6.2746530765800310 12.4162260658495516   T   T   T
  2.7220249498768756  4.6984040704782357 14.5846287494527296   T   T   T
  2.7150632145500007  0.0000000000000000  8.0000000000000000   F   F   F
  4.0725948218250014  0.7837712388936464 10.2168398316827176   F   F   F
  2.7124559498837058  1.5659324016510821 12.3959695284657325   T   T   T
  2.7497782112452609 -0.0200367716967787 14.6539678509706928   T   T   T
  4.0725948218250014  2.3513137166809397  8.0000000000000000   F   F   F
  5.4301264291000013  3.1350849555745857 10.2168398316827176   F   F   F
  4.0710367709346871  3.9195142601068444 12.3987326076210156   T   T   T
  4.0990303662814984  2.3663956512189617 14.5884497604630496   T   T   T
  5.4301264291000013  4.7026274333618794  8.0000000000000000   F   F   F
  6.7876580363750012  5.4863986722555254 10.2168398316827176   F   F   F
  5.4301491817515775  6.2734782852954964 12.3959474304132016   T   T   T
  5.4301856362582095  4.6724964103870494 14.5883957302262157   T   T   T
  5.4301264291000013  0.0000000000000000  8.0000000000000000   F   F   F
  6.7876580363750012  0.7837712388936464 10.2168398316827176   F   F   F
  5.4300215056936381  1.5657144495043891 12.3987280428522606   T   T   T
  5.4300914146914536  0.0078981457314345 14.5846312477472342   T   T   T
  6.7876580363750012  2.3513137166809397  8.0000000000000000   F   F   F
  8.1451896436500011  3.1350849555745857 10.2168398316827176   F   F   F
  6.7891835518238155  3.9196455740735532 12.3987022983718553   T   T   T
  6.7617568663075422  2.3661949506086946 14.5883977317817113   T   T   T
  8.1451896436500029  4.7026274333618794  8.0000000000000000   F   F   F
  9.5027212509250027  5.4863986722555254 10.2168398316827176   F   F   F
  8.1371395840327114  6.2747123068285058 12.4164500533493793   T   T   T
  8.1382726470191873  4.6984768649279234 14.5847455126933134   T   T   T
  1.3576518758592759  0.7836260450194064 15.9508631680924786   T   T   T

O_fcc111-3x3x4-freeze-2/Rh E_tot= -269.50896641 eV
Rh  O
 1.0000000000000000
     8.0329880858400013    0.0000000000000000    0.0000000000000000
     4.0164940429200007    6.9567717506351698    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.5392077597396820
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  7.9999999999999991   F   F   F
  1.3388313476400000  0.7729746389594633 10.1863024355738396   F   F   F
  0.0023259612911102  1.5452570543996789 12.3296492558789570   T   T   T
 -0.0140743157325347 -0.0082040808617426 14.5851002013839341   T   T   T
  1.3388313476400000  2.3189239168783899  7.9999999999999991   F   F   F
  2.6776626952800000  3.0918985558378531 10.1863024355738396   F   F   F
  1.3375944382166680  3.8581335134064942 12.3562354003080692   T   T   T
  1.3402596090937149  2.3373312163705493 14.5824409059638338   T   T   T
  2.6776626952800000  4.6378478337567799  7.9999999999999991   F   F   F
  4.0164940429200007  5.4108224727162435 10.1863024355738396   F   F   F
  2.6821094145228228  6.1862246294614813 12.3559648859646263   T   T   T
  2.6806324626486928  4.6358895369431590 14.5029122454904051   T   T   T
  2.6776626952800000  0.0000000000000000  7.9999999999999991   F   F   F
  4.0164940429200007  0.7729746389594633 10.1863024355738396   F   F   F
  2.6748204943549037  1.5442377744795106 12.3299765032339348   T   T   T
  2.6943740532100482 -0.0083241671482878 14.5824872526006342   T   T   T
```

```
  4.0164940429200007  2.3189239168783899  7.9999999999999991   F   F   F
  5.3553253905600000  3.0918985558378531 10.1863024355738396   F   F   F
  4.0134828462407111  3.8671484016394775 12.3317712798797814   T   T   T
  4.0539873054670039  2.3403763059190608 14.4990807252483975   T   T   T
  5.3553253905600000  4.6378478337567799  7.9999999999999991   F   F   F
  6.6941567381999993  5.4108224727162435 10.1863024355738396   F   F   F
  5.3559760165895254  6.1859658926806045 12.3296719327303368   T   T   T
  5.3563810201823134  4.5966492505069718 14.4995233603516169   T   T   T
  5.3553253905600000  0.0000000000000000  7.9999999999999991   F   F   F
  6.6941567381999993  0.7729746389594633 10.1863024355738396   F   F   F
  5.3558642439489947  1.5419877339511443 12.3317953098643489   T   T   T
  5.3553317663856506  0.0031582209809362 14.5028904286441449   T   T   T
  6.6941567381999993  2.3189239168783899  7.9999999999999991   F   F   F
  8.0329880858399996  3.0918985558378531 10.1863024355738396   F   F   F
  6.6962356003714056  3.8658854798018094 12.3308477194895776   T   T   T
  6.6592495787559773  2.3399523440804813 14.4997575556526250   T   T   T
  8.0329880858400013  4.6378478337567799  7.9999999999999991   F   F   F
  9.3718194334800007  5.4108224727162435 10.1863024355738396   F   F   F
  8.0265514636621074  6.1860367849288691 12.3561598862672550   T   T   T
  8.0306944661290540  4.6365197773721816 14.5034388617015164   T   T   T
  1.3402602212583117  0.7736777525000318 15.8410700546631666   T   T   T

O_fcc111-3x3x4-freeze-2/Os E_tot= -402.25407473 eV
Os  O
 1.0000000000000000
     8.1252428492400028    0.0000000000000000    0.0000000000000000
     4.0626214246200014    7.0366667193596939    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6257917084105706
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3542071415400003  0.7818518577066326 10.2114110018706405   F   F   F
  0.0083285309619157  1.5582320954974174 12.4467454375900726   T   T   T
 -0.0173968360315090 -0.0102266838150750 14.6560554412955728   T   T   T
  1.3542071415400003  2.3455555731198978  8.0000000000000000   F   F   F
  2.7084142830800007  3.1274074308265303 10.2114110018706405   F   F   F
  1.3543660168739300  3.9117762070721365 12.4150556462500425   T   T   T
  1.3540765189676520  2.3655327870943981 14.6565337472155122   T   T   T
  2.7084142830800007  4.6911111462397956  8.0000000000000000   F   F   F
  4.0626214246200014  5.4729630039464281 10.2114110018706405   F   F   F
  2.7058214380035088  6.2531592349952110 12.4146227160138878   T   T   T
  2.7087666050825869  4.6907276073223301 14.5585799598984522   T   T   T
  2.7084142830800007  0.0000000000000000  8.0000000000000000   F   F   F
  4.0626214246200014  0.7818518577066326 10.2114110018706405   F   F   F
  2.7005817814648574  1.5590184621628398 12.4474915808059876   T   T   T
  2.7258210372783021 -0.0104554575995703 14.6565382334809904   T   T   T
  4.0626214246200014  2.3455555731198978  8.0000000000000000   F   F   F
  5.4168285661600013  3.1274074308265303 10.2114110018706405   F   F   F
  4.0504871110417859  3.9163899960125548 12.4477022938642090   T   T   T
  4.0979375048454614  2.3657584889944632 14.5706402267395330   T   T   T
  5.4168285661600013  4.6911111462397956  8.0000000000000000   F   F   F
  6.7710357077000012  5.4729630039464281 10.2114110018706405   F   F   F
  5.4164044178548121  6.2645062001244218 12.4467465208027743   T   T   T
  5.4169941183118064  4.6503633004833214 14.5702944987108651   T   T   T
  5.4168285661600013  0.0000000000000000  8.0000000000000000   F   F   F
  6.7710357077000012  0.7818518577066326 10.2114110018706405   F   F   F
  5.4170600436497631  1.5493895914377371 12.4476800974425679   T   T   T
  5.4168154446988943  0.0002177220021454 14.5585944387580515   T   T   T
  6.7710357077000012  2.3455555731198978  8.0000000000000000   F   F   F
  8.1252428492400011  3.1274074308265303 10.2114110018706405   F   F   F
  6.7832513067701781  3.9161331394715666 12.4466551760216575   T   T   T
  6.7360140084570670  2.3657812118183026 14.5702442179877121   T   T   T
```

```
  8.1252428492400028  4.6911111462397956  8.0000000000000000   F   F   F
  9.4794499907800027  5.4729630039464281 10.2114110018706405   F   F   F
  8.1275989851894028  6.2534979643277628 12.4150073401452694   T   T   T
  8.1250609018755000  4.6908404510019261 14.5579294664057333   T   T   T
  1.3543275420945893  0.7816700069895163 15.9854770996722166   T   T   T

O_fcc111-3x3x4-freeze-2/Ru E_tot= -333.80692351 eV
Ru  O
 1.0000000000000000
     7.9985842258200019    0.0000000000000000    0.0000000000000000
     3.9992921129100010    6.9269771338696069    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.5069186730815076
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  7.9999999999999991   F   F   F
  1.3330973709700003  0.7696641259855118 10.1769388908814911   F   F   F
  0.0091561765739781  1.5335679172578025 12.3604644779299768   T   T   T
 -0.0158036800691518 -0.0093767562321246 14.5757448401011054   T   T   T
  1.3330973709700003  2.3089923779565353  7.9999999999999991   F   F   F
  2.6661947419400005  3.0786565039420473 10.1769388908814911   F   F   F
  1.3317664208805580  3.8555400215197264 12.3420118271788937   T   T   T
  1.3347045004972022  2.3273116054280942 14.5747534005129680   T   T   T
  2.6661947419400005  4.6179847559130707  7.9999999999999991   F   F   F
  3.9992921129100010  5.3876488818985830 10.1769388908814911   F   F   F
  2.6601009962505855  6.1535791064738392 12.3438413214380329   T   T   T
  2.6699769707579852  4.6130050984750186 14.4472096914838239   T   T   T
  2.6661947419400005  0.0000000000000000  7.9999999999999991   F   F   F
  3.9992921129100010  0.7696641259855118 10.1769388908814911   F   F   F
  2.6559377567410229  1.5333331090168494 12.3601359465925515   T   T   T
  2.6830794506725324 -0.0081646414027513 14.5747549820038440   T   T   T
  3.9992921129100010  2.3089923779565353  7.9999999999999991   F   F   F
  5.3323894838800010  3.0786565039420473 10.1769388908814911   F   F   F
  3.9869122454218662  3.8554659883743576 12.3642172003848199   T   T   T
  4.0335887121959413  2.3284186272868546 14.4532331507156488   T   T   T
  5.3323894838800010  4.6179847559130707  7.9999999999999991   F   F   F
  6.6654868548500010  5.3876488818985830 10.1769388908814911   F   F   F
  5.3320141683536706  6.1680289834473729 12.3603963613825591   T   T   T
  5.3309266156969164  4.5776989164901609 14.4534793445258334   T   T   T
  5.3323894838800010  0.0000000000000000  7.9999999999999991   F   F   F
  6.6654868548500010  0.7696641259855118 10.1769388908814911   F   F   F
  5.3326087405983102  1.5248392513657156 12.3642958242677672   T   T   T
  5.3304146370160286  0.0054355829260107 14.4471477833503705   T   T   T
  6.6654868548500010  2.3089923779565353  7.9999999999999991   F   F   F
  7.9985842258200002  3.0786565039420473 10.1769388908814911   F   F   F
  6.6745787583466134  3.8534946956833784 12.3615534937805887   T   T   T
  6.6301608831644128  2.3275908146568871 14.4534357619583744   T   T   T
  7.9985842258200019  4.6179847559130707  7.9999999999999991   F   F   F
  9.3316815967900020  5.3876488818985830 10.1769388908814911   F   F   F
  8.0042221415033215  6.1524877719542239 12.3419485508442275   T   T   T
  7.9891589374759988  4.6125533217851284 14.4457869601549067   T   T   T
  1.3339438080790773  0.7698624276476967 15.8519599783248939   T   T   T

fcc111-1x1x4-freeze-2_kpts.12_clean/Au E_tot= -14.18732425 eV
Au
 1.0000000000000000
     2.8987517104700005    0.0000000000000000    0.0000000000000000
     1.4493758552350002    2.5103926205306140    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.1272073742742990
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
```

```
  1.4493758552350002  0.8367975401768712 10.3668208605571550   F   F   F
  0.0000127707523299  1.6735413370852861 12.7136800773439660   T   T   T
  0.0000365345881270 -0.0001864866281991 15.1270706599885845   T   T   T

fcc111-1x1x4-freeze-2_kpts.12_clean/Ag E_tot= -11.64154158 eV
Ag
 1.0000000000000000
     2.8805270519500010    0.0000000000000000    0.0000000000000000
     1.4402635259750005    2.4946096032769978    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.0600324704191415
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.4402635259750005  0.8315365344256658 10.3519404891869975   F   F   F
  0.0000067779213152  1.6630016845745994 12.6786594352751614   T   T   T
  0.0000473148696597 -0.0002310376236870 15.0480129802377007   T   T   T

fcc111-1x1x4-freeze-2_kpts.12_clean/Cu E_tot= -15.44946271 eV
Cu
 1.0000000000000000
     2.5237696367300004    0.0000000000000000    0.0000000000000000
     1.2618848183650002    2.1856486187080040    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.1807007091391455
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.2618848183650002  0.7285495395693345 10.0606492794392555   F   F   F
  0.0000110856630822  1.4570813329028303 12.1091457336738557   T   T   T
  0.0000134339467938 -0.0000260587542602 14.1807007091391490   T   T   T

fcc111-1x1x4-freeze-2_kpts.12_clean/Pt E_tot= -25.45958694 eV
Pt
 1.0000000000000000
     2.7704533654200003    0.0000000000000000    0.0000000000000000
     1.3852266827100002    2.3992829944538121    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.8063440971582203
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  7.9999999999999991   F   F   F
  1.3852266827100002  0.7997609981512707 10.2620657004851399   F   F   F
  0.0000194682629634  1.5994287163884102 12.5138221423953997   T   T   T
  0.0000554610620094 -0.0002567219139211 14.8121954256765722   T   T   T

fcc111-1x1x4-freeze-2_kpts.12_clean/Pd E_tot= -21.42628724 eV
Pd
 1.0000000000000000
     2.7479812319000003    0.0000000000000000    0.0000000000000000
     1.3739906159500002    2.3798215559482565    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.7524988809318387
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3739906159500002  0.7932738519827521 10.2437172802999115   F   F   F
 -0.0000412484852474  1.5867567397580127 12.4811843633316251   T   T   T
 -0.0001081482455568  0.0002601196696727 14.7521834032834942   T   T   T

fcc111-1x1x4-freeze-2_kpts.12_clean/Ni E_tot= -21.72917745 eV
Ni
 1.0000000000000000
```

```
     2.4538580817700004    0.0000000000000000    0.0000000000000000
     1.2269290408850002    2.1251034360945718    0.0000000000000000
     0.0000000000000000    0.0000000000000000   21.9386693776092692
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.2269290408850002  0.7083678120315239 10.0035667338470748   F   F   F
  0.0000217008732468  1.4166601283466715 12.0203398098739900   T   T   T
  0.0000557376919081 -0.0002342453885513 14.0385884145876609   T   T   T

fcc111-1x1x4-freeze-2_kpts.12_clean/Ir E_tot= -35.66388056 eV
Ir
 1.0000000000000000
     2.7150632145500007    0.0000000000000000    0.0000000000000000
     1.3575316072750003    2.3513137166809397    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.5952820915883947
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3575316072750003  0.7837712388936464 10.2168398316827158   F   F   F
  0.0000361969898318  1.5675354213864119 12.4024364598310193   T   T   T
 -0.0000192160715005 -0.0000282284998758 14.5952820915883947   T   T   T

fcc111-1x1x4-freeze-2_kpts.12_clean/Rh E_tot= -29.16025102 eV
Rh
 1.0000000000000000
     2.6776626952800004    0.0000000000000000    0.0000000000000000
     1.3388313476400002    2.3189239168783899    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.5084435367048670
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  7.9999999999999991   F   F   F
  1.3388313476400002  0.7729746389594633 10.1863024355738396   F   F   F
  0.0000192608838614  1.5459131865216134 12.3311167714607901   T   T   T
  0.0000543656814575 -0.0000369292772035 14.5037398062264256   T   T   T

fcc111-1x1x4-freeze-2_kpts.12_clean/Os E_tot= -43.85459559 eV
Os
 1.0000000000000000
     2.7084142830800007    0.0000000000000000    0.0000000000000000
     1.3542071415400003    2.3455555731198978    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.5835846887241836
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3542071415400003  0.7818518577066326 10.2114110018706405   F   F   F
 -0.0000075180692118  1.5637416064611334 12.4470857466151088   T   T   T
 -0.0000324330983592  0.0000296073564408 14.5835846887241871   T   T   T

fcc111-1x1x4-freeze-2_kpts.12_clean/Ru E_tot= -36.21752763 eV
Ru
 1.0000000000000000
     2.6661947419400005    0.0000000000000000    0.0000000000000000
     1.3330973709700003    2.3089923779565353    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.4736071478595534
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
```

```
  1.3330973709700003  0.7696641259855117 10.1769388908814911   F   F   F
  0.0000671674051825  1.5389315674693005 12.3651954411950911   T   T   T
  0.0000435347941286 -0.0000899905455667 14.4727522226435337   T   T   T

O_fcc100-3x3x4-freeze-2/Au E_tot= -129.75232413 eV
Au  O
 1.0000000000000000
     8.6962551314100036    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6962551314100036    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.4574584900542185
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.4493758552350002  1.4493758552350002 10.0497269914494414   F   F   F
 -0.0073262080549071 -0.0001186217740757 12.0964572591946116   T   T   T
  1.4438551107316833  1.4183742135050879 14.1660873028535939   T   T   T
  0.0000000000000000  2.8987517104700005  8.0000000000000000   F   F   F
  1.4493758552350002  4.3481275657050018 10.0497269914494414   F   F   F
  0.0197995896228338  2.9075416688235323 12.1199428474206812   T   T   T
  1.2878091203723565  4.3481909710559146 14.3233969537082544   T   T   T
  0.0000000000000000  5.7975034209400009  8.0000000000000000   F   F   F
  1.4493758552350002  7.2468792761750009 10.0497269914494414   F   F   F
  0.0197678824487699  5.7883749175591594 12.1200224045114329   T   T   T
  1.4440825761124105  7.2774950728144177 14.1662668871940358   T   T   T
  2.8987517104700005  0.0000000000000000  8.0000000000000000   F   F   F
  4.3481275657050018  1.4493758552350002 10.0497269914494414   F   F   F
  2.8988124998437530  0.0001736899618118 12.0990477228914717   T   T   T
  4.3536311152809146  1.4183533182105865 14.1661215242181093   T   T   T
  2.8987517104700005  2.8987517104700005  8.0000000000000000   F   F   F
  4.3481275657050018  4.3481275657050018 10.0497269914494414   F   F   F
  2.8987631136181711  2.9303853573757230 12.1302545650357825   T   T   T
  4.5096144016303006  4.3482237473871370 14.3234369837022690   T   T   T
  2.8987517104700005  5.7975034209400009  8.0000000000000000   F   F   F
  4.3481275657050018  7.2468792761750009 10.0497269914494414   F   F   F
  2.8987013975778231  5.7658189577988006 12.1304667860859468   T   T   T
  4.3533284978876905  7.2774769981872574 14.1663091146205922   T   T   T
  5.7975034209400009  0.0000000000000000  8.0000000000000000   F   F   F
  7.2468792761750009  1.4493758552350002 10.0497269914494414   F   F   F
  5.8047768803092392 -0.0001528734081652 12.0964434663851357   T   T   T
  7.2468576152600361  1.4399015050690778 14.1765261815018384   T   T   T
  5.7975034209400009  2.8987517104700005  8.0000000000000000   F   F   F
  7.2468792761750009  4.3481275657050018 10.0497269914494414   F   F   F
  5.7777022000802569  2.9075574834088624 12.1199133142452382   T   T   T
  7.2468266783875581  4.3479366871893275 14.1452620787432295   T   T   T
  5.7975034209400009  5.7975034209400009  8.0000000000000000   F   F   F
  7.2468792761750009  7.2468792761750009 10.0497269914494414   F   F   F
  5.7776245200030694  5.7883751212020051 12.1200377767575009   T   T   T
  7.2467978375701882  7.2556616646978513 14.1767492965709163   T   T   T
  2.8987138006612470  4.3451145253714918 15.5641049485702556   T   T   T

O_fcc100-3x3x4-freeze-2/Ag E_tot= -108.31895873 eV
Ag  O
 1.0000000000000000
     8.6415811558500017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6415811558500017    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.0478776095053135
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  7.9999999999999991   F   F   F
  1.4402635259750003  1.4402635259750003 10.0368402118251403   F   F   F
  0.0077020112761343  0.0077504748868246 12.1037776893476536   T   T   T
```

```
  1.3973765699882359  1.3971898128171145 14.1811416203909033   T   T   T
  0.0000000000000000  2.8805270519500006  7.9999999999999991   F   F   F
  1.4402635259750003  4.3207905779250009 10.0368402118251403   F   F   F
  0.0124795049963794  2.8804637389330345 12.0941388711370728   T   T   T
  1.3974738289164437  4.3631228043937380 14.1813074973573610   T   T   T
  0.0000000000000000  5.7610541039000012  7.9999999999999991   F   F   F
  1.4402635259750003  7.2013176298750006 10.0368402118251403   F   F   F
  0.0078672862523399  5.7531914282580967 12.1037453535540003   T   T   T
  1.4303139599616217  7.2006941434922922 14.1198056496851549   T   T   T
  2.8805270519500006  0.0000000000000000  7.9999999999999991   F   F   F
  4.3207905779250009  1.4402635259750003 10.0368402118251403   F   F   F
  2.8805229352097865  0.0122665807031019 12.0941200827621156   T   T   T
  4.3634338009263862  1.3972153174400002 14.1811739303509654   T   T   T
  2.8805270519500006  2.8805270519500006  7.9999999999999991   F   F   F
  4.3207905779250009  4.3207905779250009 10.0368402118251403   F   F   F
  2.8804667301361260  2.8803077092440752 12.0435895320345825   T   T   T
  4.3632659998399621  4.3631112730495616 14.1813360752877902   T   T   T
  2.8805270519500006  5.7610541039000012  7.9999999999999991   F   F   F
  4.3207905779250009  7.2013176298750006 10.0368402118251403   F   F   F
  2.8805559246838324  5.7480815840406656 12.0943246658627999   T   T   T
  4.3308012706162780  7.2006865884262927 14.1197303442579472   T   T   T
  5.7610541039000012  0.0000000000000000  7.9999999999999991   F   F   F
  7.2013176298750006  1.4402635259750003 10.0368402118251403   F   F   F
  5.7532645532844544  0.0077998472587683 12.1037580502513755   T   T   T
  7.2011234651215377  1.4302663489169043 14.1198074251561856   T   T   T
  5.7610541039000012  2.8805270519500006  7.9999999999999991   F   F   F
  7.2013176298750006  4.3207905779250009 10.0368402118251403   F   F   F
  5.7483658049467907  2.8805154552053325 12.0941721181352673   T   T   T
  7.2011059085969649  4.3307081784906840 14.1196637967787861   T   T   T
  5.7610541039000012  5.7610541039000012  7.9999999999999991   F   F   F
  7.2013176298750006  7.2013176298750006 10.0368402118251403   F   F   F
  5.7532047197758569  5.7531500550953929 12.1037522456684474   T   T   T
  7.2013062572343651  7.2012650298553211 14.1495299498339264   T   T   T
  2.8803669986874687  2.8800077603248355 14.9782802556542958   T   T   T

O_fcc100-3x3x4-freeze-2/Cu E_tot= -142.75935626 eV
Cu  O
 1.0000000000000000
     7.5713089101900026    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.5713089101900026    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.4927628111072657
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.2618848183650002  1.2618848183650002  9.7845746242844935   F   F   F
  0.0086229230134832  0.0106987783567404 11.6126346188493681   T   T   T
  1.2409825702236488  1.2400534298945434 13.4376924547303016   T   T   T
  0.0000000000000000  2.5237696367300004  8.0000000000000000   F   F   F
  1.2618848183650002  3.7856544550950013  9.7845746242844935   F   F   F
  0.0131129533107994  2.5251553489255780 11.6004223344560486   T   T   T
  1.2378199844168347  3.8087856951211378 13.4379569914399628   T   T   T
  0.0000000000000000  5.0475392734600009  8.0000000000000000   F   F   F
  1.2618848183650002  6.3094240918250009  9.7845746242844935   F   F   F
  0.0085351950833363  5.0392421329146693 11.6125684575957742   T   T   T
  1.2580372251281837  6.3097010285181225 13.3539653617058125   T   T   T
  2.5237696367300004  0.0000000000000000  8.0000000000000000   F   F   F
  3.7856544550950013  1.2618848183650002  9.7845746242844935   F   F   F
  2.5233932300512638  0.0141654952858994 11.6015535262132126   T   T   T
  3.8107943353683864  1.2413577606675450 13.4387010205917896   T   T   T
  2.5237696367300004  2.5237696367300004  8.0000000000000000   F   F   F
  3.7856544550950013  3.7856544550950013  9.7845746242844935   F   F   F
  2.5238470421169903  2.5241582710162649 11.5352564927610004   T   T   T
```

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  3.8075318326938188  3.8106903646514274 13.4359955967406037   T   T   T
  2.5237696367300004  5.0475392734600009  8.0000000000000000   F   F   F
  3.7856544550950013  6.3094240918250009  9.7845746242844935   F   F   F
  2.5226624670124860  5.0352627041537001 11.6009286673928091   T   T   T
  3.7872472798185330  6.3105973337359416 13.3541698847870496   T   T   T
  5.0475392734600009  0.0000000000000000  8.0000000000000000   F   F   F
  6.3094240918250009  1.2618848183650002  9.7845746242844935   F   F   F
  5.0369521477566224  0.0115169904006664 11.6125628110298713   T   T   T
  6.3100225632868234  1.2635761878153760 13.3534492098873052   T   T   T
  5.0475392734600009  2.5237696367300004  8.0000000000000000   F   F   F
  6.3094240918250009  3.7856544550950013  9.7845746242844935   F   F   F
  5.0349457482646418  2.5257463714068442 11.6012324704135796   T   T   T
  6.3064411720978741  3.7937015121429107 13.3538937399962787   T   T   T
  5.0475392734600009  5.0475392734600009  8.0000000000000000   F   F   F
  6.3094240918250009  6.3094240918250009  9.7845746242844935   F   F   F
  5.0371022045221450  5.0408050817408974 11.6117087688210283   T   T   T
  6.3077283592675180  6.3133365602227851 13.3781196779091616   T   T   T
  2.5241485179762537  2.5254701022448955 14.2533338774570151   T   T   T

O_fcc100-3x3x4-freeze-2/Pt E_tot= -229.38809573 eV
Pt  O
 1.0000000000000000
     8.3113600962600014    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.3113600962600014    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.1273924208916775
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3852266827100002  1.3852266827100002  9.9590063616495765   F   F   F
 -0.0090756171790515 -0.0001389037468755 11.8753557790470357   T   T   T
  1.3798608752533428  1.3538544429957151 13.8197629874141121   T   T   T
  0.0000000000000000  2.7704533654200003  8.0000000000000000   F   F   F
  1.3852266827100002  4.1556800481300007  9.9590063616495765   F   F   F
  0.0075274443914658  2.7858993154259037 11.9247719419375642   T   T   T
  1.2813909046876328  4.1554129219331388 13.9646650194934274   T   T   T
  0.0000000000000000  5.5409067308400006  8.0000000000000000   F   F   F
  1.3852266827100002  6.9261334135499997  9.9590063616495765   F   F   F
  0.0074526185462624  5.5250917362860354 11.9248891883715871   T   T   T
  1.3796705759711121  6.9569551259112936 13.8197941503223518   T   T   T
  2.7704533654200003  0.0000000000000000  8.0000000000000000   F   F   F
  4.1556800481300007  1.3852266827100002  9.9590063616495765   F   F   F
  2.7704349519374416 -0.0001856525147347 11.8759973967030223   T   T   T
  4.1610531447277772  1.3538597661159002 13.8197157114136093   T   T   T
  2.7704533654200003  2.7704533654200003  8.0000000000000000   F   F   F
  4.1556800481300007  4.1556800481300007  9.9590063616495765   F   F   F
  2.7704694899605551  2.7863528720158901 11.9195354428860334   T   T   T
  4.2594929121905771  4.1554846235396212 13.9646330444883091   T   T   T
  2.7704533654200003  5.5409067308400006  8.0000000000000000   F   F   F
  4.1556800481300007  6.9261334135499997  9.9590063616495765   F   F   F
  2.7704397320182998  5.5247486641925940 11.9195738660764441   T   T   T
  4.1611592373769399  6.9569884743900108 13.8197516804388236   T   T   T
  5.5409067308400006  0.0000000000000000  8.0000000000000000   F   F   F
  6.9261334135499997  1.3852266827100002  9.9590063616495765   F   F   F
  5.5499822795239968 -0.0001600836557525 11.8753604228558380   T   T   T
  6.9261577130515439  1.3704965776071909 13.8425151157046624   T   T   T
  5.5409067308400006  2.7704533654200003  8.0000000000000000   F   F   F
  6.9261334135499997  4.1556800481300007  9.9590063616495765   F   F   F
  5.5334382855860262  2.7859381372497554 11.9247883899859985   T   T   T
  6.9261412558242501  4.1551892732163189 13.8911710503090884   T   T   T
  5.5409067308400006  5.5409067308400006  8.0000000000000000   F   F   F
  6.9261334135499997  6.9261334135499997  9.9590063616495765   F   F   F
  5.5334317259776507  5.5250595610185051 11.9249213283643645   T   T   T
```

```
  6.9260957989115655  6.9404330996875476 13.8424955706147355   T   T   T
  2.7704557914849079  4.1547300486810839 15.2113006918514468   T   T   T

O_fcc100-3x3x4-freeze-2/Pd E_tot= -195.33553394 eV
Pd  O
 1.0000000000000000
     8.2439436957000023    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.2439436957000023    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.7235735149711147
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3739906159500004  1.3739906159500004  9.9431161636498544   F   F   F
  0.0070440238760684  0.0069094556220995 11.9178983167470722   T   T   T
  1.3709519149837426  1.3706701764876204 13.8667634908333213   T   T   T
  0.0000000000000000  2.7479812319000008  8.0000000000000000   F   F   F
  1.3739906159500004  4.1219718478500011  9.9431161636498544   F   F   F
 -0.0133717202528683  2.7476227780697879 11.8832631217371265   T   T   T
  1.3690761953487154  4.1259495596536606 13.8641884486834499   T   T   T
  0.0000000000000000  5.4959624638000015  8.0000000000000000   F   F   F
  1.3739906159500004  6.8699530797500010  9.9431161636498544   F   F   F
  0.0062846465239485  5.4895537948116306 11.9182600354547983   T   T   T
  1.3738140837780393  6.8703707436250401 13.8673919460074799   T   T   T
  2.7479812319000008  0.0000000000000000  8.0000000000000000   F   F   F
  4.1219718478500011  1.3739906159500004  9.9431161636498544   F   F   F
  2.7477438678325359 -0.0135898713549679 11.8832936991817704   T   T   T
  4.1261276515131984  1.3686661852959925 13.8641862928769193   T   T   T
  2.7479812319000008  2.7479812319000008  8.0000000000000000   F   F   F
  4.1219718478500011  4.1219718478500011  9.9431161636498544   F   F   F
  2.7475965419100605  2.7474028963038406 11.8322784460256116   T   T   T
  4.1249330789796215  4.1247837776741472 13.8664190734956598   T   T   T
  2.7479812319000008  5.4959624638000015  8.0000000000000000   F   F   F
  4.1219718478500011  6.8699530797500010  9.9431161636498544   F   F   F
  2.7470598559801078  5.5074483492171034 11.8838548257479761   T   T   T
  4.1220331088532829  6.8680385641735455 13.8652316832808928   T   T   T
  5.4959624638000015  0.0000000000000000  8.0000000000000000   F   F   F
  6.8699530797500010  1.3739906159500004  9.9431161636498544   F   F   F
  5.4896812440473850  0.0061345082375283 11.9182535547845827   T   T   T
  6.8706666360998003  1.3737013703674967 13.8673996647621198   T   T   T
  5.4959624638000015  2.7479812319000008  8.0000000000000000   F   F   F
  6.8699530797500010  4.1219718478500011  9.9431161636498544   F   F   F
  5.5074793561031283  2.7470240815632128 11.8838600505013350   T   T   T
  6.8684550050936588  4.1218870083977937 13.8652395911587156   T   T   T
  5.4959624638000015  5.4959624638000015  8.0000000000000000   F   F   F
  6.8699530797500010  6.8699530797500010  9.9431161636498544   F   F   F
  5.4891349134301919  5.4889697986203609 11.9168155854171349   T   T   T
  6.8700257911742941  6.8699594763340537 13.8673869351878700   T   T   T
  2.7492408742410221  2.7488020364765378 14.7623372137917617   T   T   T

O_fcc100-3x3x4-freeze-2/Ni E_tot= -198.94237779 eV
Ni  O
 1.0000000000000000
     7.3615742453100017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.3615742453100017    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.0039330023659296
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.2269290408850002  1.2269290408850002  9.7351396896889799   F   F   F
  0.0061624916862387  0.0059370999475643 11.5175355725378648   T   T   T
  1.2230236460654864  1.2228978998406557 13.2817298471611966   T   T   T
```

```
  0.0000000000000000  2.4538580817700004  8.0000000000000000   F   F   F
  1.2269290408850002  3.6807871226550009  9.7351396896889799   F   F   F
  0.0004652886999826  2.4536644049372685 11.5010310697581328   T   T   T
  1.2228666147523035  3.6844005165283873 13.2815979977554548   T   T   T
  0.0000000000000000  4.9077161635400008  8.0000000000000000   F   F   F
  1.2269290408850002  6.1346452044250004  9.7351396896889799   F   F   F
  0.0061735703529732  4.9012059615805459 11.5175164452691021   T   T   T
  1.2267063779637846  6.1344962237910723 13.2132835279116883   T   T   T
  2.4538580817700004  0.0000000000000000  8.0000000000000000   F   F   F
  3.6807871226550009  1.2269290408850002  9.7351396896889799   F   F   F
  2.4538385492604817  0.0004271593956788 11.5010045406607659   T   T   T
  3.6844484463151992  1.2228838431146181 13.2815845556352752   T   T   T
  2.4538580817700004  2.4538580817700004  8.0000000000000000   F   F   F
  3.6807871226550009  3.6807871226550009  9.7351396896889799   F   F   F
  2.4537908203027747  2.4537363414193227 11.4358450110416392   T   T   T
  3.6847276163531237  3.6845158245164593 13.2814873271545082   T   T   T
  2.4538580817700004  4.9077161635400008  8.0000000000000000   F   F   F
  3.6807871226550009  6.1346452044250004  9.7351396896889799   F   F   F
  2.4538231061537457  4.9070359630573339 11.5011096111184710   T   T   T
  3.6810295685758101  6.1344920477626523 13.2132968202379093   T   T   T
  4.9077161635400008  0.0000000000000000  8.0000000000000000   F   F   F
  6.1346452044250004  1.2269290408850002  9.7351396896889799   F   F   F
  4.9014700674245635  0.0059600677817346 11.5175074452197599   T   T   T
  6.1345772226647721  1.2267220194682633 13.2132057072350655   T   T   T
  4.9077161635400008  2.4538580817700004  8.0000000000000000   F   F   F
  6.1346452044250004  3.6807871226550009  9.7351396896889799   F   F   F
  4.9071818067040063  2.4536662084515122 11.5009786598962549   T   T   T
  6.1345889539191818  3.6810808648656881 13.2133804034930940   T   T   T
  4.9077161635400008  4.9077161635400008  8.0000000000000000   F   F   F
  6.1346452044250004  6.1346452044250004  9.7351396896889799   F   F   F
  4.9014307157542483  4.9012512509326722 11.5174904153072557   T   T   T
  6.1346173183600605  6.1344532870931490 13.2147065163574613   T   T   T
  2.4537958642488218  2.4535836481866333 14.1324429605241519   T   T   T

O_fcc100-3x3x4-freeze-2/Ir E_tot= -318.44203382 eV
Ir  O
 1.0000000000000000
     8.1451896436500029    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1451896436500029    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.9848932377505690
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3575316072750003  1.3575316072750003  9.9198396103584514   F   F   F
 -0.0151485191385814 -0.0001198644227139 11.8227615733808609   T   T   T
  1.3489506256947326  1.3191293344310213 13.6901063104103535   T   T   T
  0.0000000000000000  2.7150632145500007  8.0000000000000000   F   F   F
  1.3575316072750003  4.0725948218250014  9.9198396103584514   F   F   F
  0.0236663471850999  2.7317297213940193 11.8733862279622961   T   T   T
  1.2846466650466728  4.0724126418518454 13.8174292754524259   T   T   T
  0.0000000000000000  5.4301264291000013  8.0000000000000000   F   F   F
  1.3575316072750003  6.7876580363750012  9.9198396103584514   F   F   F
  0.0236409643077356  5.4132199284487559 11.8733528180676924   T   T   T
  1.3490567464792615  6.8255393262149973 13.6901161480468794   T   T   T
  2.7150632145500007  0.0000000000000000  8.0000000000000000   F   F   F
  4.0725948218250014  1.3575316072750003  9.9198396103584514   F   F   F
  2.7149421312832542 -0.0001133831610596 11.8406605119696131   T   T   T
  4.0808527604329266  1.3189031284915156 13.6902831570395538   T   T   T
  2.7150632145500007  2.7150632145500007  8.0000000000000000   F   F   F
  4.0725948218250014  4.0725948218250014  9.9198396103584514   F   F   F
  2.7151747593897193  2.7155490033784120 11.8585210432063395   T   T   T
  4.1463353143117097  4.0723977283945398 13.8172059572974995   T   T   T
```

```
  2.7150632145500007  5.4301264291000013  8.0000000000000000   F   F   F
  4.0725948218250014  6.7876580363750012  9.9198396103584514   F   F   F
  2.7151895384816469  5.4293875996264340 11.8584244986433518   T   T   T
  4.0807478444410954  6.8257685866074569 13.6903136101915770   T   T   T
  5.4301264291000013  0.0000000000000000  8.0000000000000000   F   F   F
  6.7876580363750012  1.3575316072750003  9.9198396103584514   F   F   F
  5.4451805271968317 -0.0001263524932410 11.8228320941923108   T   T   T
  6.7878276399340844  1.3443428169278995 13.6899941867908286   T   T   T
  5.4301264291000013  2.7150632145500007  8.0000000000000000   F   F   F
  6.7876580363750012  4.0725948218250014  9.9198396103584514   F   F   F
  5.4063424630215691  2.7316932056775594 11.8730939889649800   T   T   T
  6.7877061726315704  4.0724778336493621 13.6981354716358510   T   T   T
  5.4301264291000013  5.4301264291000013  8.0000000000000000   F   F   F
  6.7876580363750012  6.7876580363750012  9.9198396103584514   F   F   F
  5.4063730600182849  5.4132791962741198 11.8730809614359227   T   T   T
  6.7878462819422163  6.8005792179297035 13.6899933295981793   T   T   T
  2.7159166544927817  4.0711935630243792 15.1186457744541620   T   T   T

O_fcc100-3x3x4-freeze-2/Rh E_tot= -263.14572928 eV
Rh  O
 1.0000000000000000
     8.0329880858400013    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.0329880858400013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.5515229038019598
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  7.9999999999999991   F   F   F
  1.3388313476400000  1.3388313476400000  9.8933934495627351   F   F   F
  0.0074000272898386  0.0073359506492004 11.8001680623932170   T   T   T
  1.3421384351633601  1.3419805082564882 13.6848761222741455   T   T   T
  0.0000000000000000  2.6776626952800000  7.9999999999999991   F   F   F
  1.3388313476400000  4.0164940429200007  9.8933934495627351   F   F   F
 -0.0103078283163376  2.6764818315478531 11.7907331841693104   T   T   T
  1.3422217101585969  4.0142138970092613 13.6825389854010044   T   T   T
  0.0000000000000000  5.3553253905600000  7.9999999999999991   F   F   F
  1.3388313476400000  6.6941567381999993  9.8933934495627351   F   F   F
  0.0080703774895521  5.3497414840191491 11.8020512845106200   T   T   T
  1.3265812629227713  6.6940454219333176 13.6393798884087030   T   T   T
  2.6776626952800000  0.0000000000000000  7.9999999999999991   F   F   F
  4.0164940429200007  1.3388313476400000  9.8933934495627351   F   F   F
  2.6762495495255036 -0.0103199805145177 11.7906857565106300   T   T   T
  4.0145491789884611  1.3419827984667094 13.6826372663758953   T   T   T
  2.6776626952800000  2.6776626952800000  7.9999999999999991   F   F   F
  4.0164940429200007  4.0164940429200007  9.8933934495627351   F   F   F
  2.6757515937113565  2.6756604743800012 11.7349061043802685   T   T   T
  4.0124380609375701  4.0122728470743443 13.6783237824329298   T   T   T
  2.6776626952800000  5.3553253905600000  7.9999999999999991   F   F   F
  4.0164940429200007  6.6941567381999993  9.8933934495627351   F   F   F
  2.6772015228821568  5.3664727395151193 11.7881783387132018   T   T   T
  4.0294759968191709  6.6933894214948095 13.6366268609330792   T   T   T
  5.3553253905600000  0.0000000000000000  7.9999999999999991   F   F   F
  6.6941567381999993  1.3388313476400000  9.8933934495627351   F   F   F
  5.3497285983806204  0.0079026857672684 11.8020435039601441   T   T   T
  6.6941814522980172  1.3265149058574974 13.6394705382280002   T   T   T
  5.3553253905600000  2.6776626952800000  7.9999999999999991   F   F   F
  6.6941567381999993  4.0164940429200007  9.8933934495627351   F   F   F
  5.3666025267066058  2.6770752134652773 11.7881710964160380   T   T   T
  6.6935520224256306  4.0294061249224313 13.6366569519775975   T   T   T
  5.3553253905600000  5.3553253905600000  7.9999999999999991   F   F   F
  6.6941567381999993  6.6941567381999993  9.8933934495627351   F   F   F
  5.3445976619477760  5.3444838614420807 11.7978777421651024   T   T   T
  6.6919700412943159  6.6919077109257579 13.6423159984742473   T   T   T
```

```
  2.6788308538923546  2.6782579389961234 14.6662638429134695   T   T   T

O_fcc100-3x3x4-freeze-2/Os E_tot= -391.15618585 eV
Os  O
 1.0000000000000000
     8.1252428492400028    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1252428492400028    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.9677878988346329
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3542071415400003  1.3542071415400003  9.9151381058283707   F   F   F
  0.0058534397443359  0.0000277040474830 11.8862126941455788   T   T   T
  1.3349034576979997  1.3095502316215102 13.6797339545603922   T   T   T
  0.0000000000000000  2.7084142830800007  8.0000000000000000   F   F   F
  1.3542071415400003  4.0626214246200014  9.9151381058283707   F   F   F
  0.0009261950573850  2.7157147867389071 11.8907792349037873   T   T   T
  1.3058125990556555  4.0625515756703958 13.7619554970030489   T   T   T
  0.0000000000000000  5.4168285661600013  8.0000000000000000   F   F   F
  1.3542071415400003  6.7710357077000012  9.9151381058283707   F   F   F
  0.0008914335234751  5.4096641755148518 11.8905637250788914   T   T   T
  1.3349899944353680  6.8153993702331270 13.6797684236231323   T   T   T
  2.7084142830800007  0.0000000000000000  8.0000000000000000   F   F   F
  4.0626214246200014  1.3542071415400003  9.9151381058283707   F   F   F
  2.7083859586287136 -0.0002194315689432 11.8675158262008136   T   T   T
  4.0823499937870089  1.3099779158773495 13.6794047074480520   T   T   T
  2.7084142830800007  2.7084142830800007  8.0000000000000000   F   F   F
  4.0626214246200014  4.0626214246200014  9.9151381058283707   F   F   F
  2.7081073369459858  2.7054624065988060 11.9105799747302434   T   T   T
  4.1094945365082598  4.0625047484796735 13.7625530265947020   T   T   T
  2.7084142830800007  5.4168285661600013  8.0000000000000000   F   F   F
  4.0626214246200014  6.7710357077000012  9.9151381058283707   F   F   F
  2.7081036539988128  5.4195293395746287 11.9105404587663273   T   T   T
  4.0823340718447119  6.8149061522008711 13.6794252939193228   T   T   T
  5.4168285661600013  0.0000000000000000  8.0000000000000000   F   F   F
  6.7710357077000012  1.3542071415400003  9.9151381058283707   F   F   F
  5.4115760682611818  0.0000661424668999 11.8856406845062921   T   T   T
  6.7710977421809737  1.3508455644253954 13.6762499545920235   T   T   T
  5.4168285661600013  2.7084142830800007  8.0000000000000000   F   F   F
  6.7710357077000012  4.0626214246200014  9.9151381058283707   F   F   F
  5.4156655990731428  2.7168159499232929 11.8914553777633234   T   T   T
  6.7710808910737699  4.0627221432896894 13.6643608564754455   T   T   T
  5.4168285661600013  5.4168285661600013  8.0000000000000000   F   F   F
  6.7710357077000012  6.7710357077000012  9.9151381058283707   F   F   F
  5.4156924373668165  5.4085433577716691 11.8912421507263346   T   T   T
  6.7711212591478729  6.7743988030496407 13.6761884001389493   T   T   T
  2.7083751159122609  4.0604382912202901 15.1305574992351506   T   T   T

O_fcc100-3x3x4-freeze-2/Ru E_tot= -326.29532018 eV
Ru  O
 1.0000000000000000
     7.9985842258200019    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.9985842258200019    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.5234638958099609
  36   1
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3330973709700003  1.3330973709700003  9.8852843819896918   F   F   F
  0.0040621638765814  0.0039178035142118 11.8337429865122949   T   T   T
  1.3497886149971750  1.3497670942167936 13.6331962533743081   T   T   T
  0.0000000000000000  2.6661947419400005  8.0000000000000000   F   F   F
```

```
  1.3330973709700003  3.9992921129100010  9.8852843819896918   F   F   F
 -0.0122476652367730  2.6679557668743556 11.8259884334561143   T   T   T
  1.3445400512980286  3.9847273948413573 13.6303007177683888   T   T   T
  0.0000000000000000  5.3323894838800010  8.0000000000000000   F   F   F
  1.3330973709700003  6.6654868548500010  9.8852843819896918   F   F   F
  0.0029875913519342  5.3281339009042581 11.8326256394805576   T   T   T
  1.3283705691629979  6.6676374212714569 13.5898685179621115   T   T   T
  2.6661947419400005  0.0000000000000000  8.0000000000000000   F   F   F
  3.9992921129100010  1.3330973709700003  9.8852843819896918   F   F   F
  2.6680122176210261 -0.0121889760218033 11.8260031900938092   T   T   T
  3.9845955064631684  1.3444865033646374 13.6303840589183398   T   T   T
  2.6661947419400005  2.6661947419400005  8.0000000000000000   F   F   F
  3.9992921129100010  3.9992921129100010  9.8852843819896918   F   F   F
  2.6662913151267138  2.6664068762360333 11.7644050982515846   T   T   T
  3.9812988388287400  3.9813399643896310 13.6335364467101403   T   T   T
  2.6661947419400005  5.3323894838800010  8.0000000000000000   F   F   F
  3.9992921129100010  6.6654868548500010  9.8852843819896918   F   F   F
  2.6656242930742242  5.3448610211530276 11.8283876222387949   T   T   T
  4.0041034971879537  6.6632188850789777 13.5916438009545963   T   T   T
  5.3323894838800010  0.0000000000000000  8.0000000000000000   F   F   F
  6.6654868548500010  1.3330973709700003  9.8852843819896918   F   F   F
  5.3282163741689388  0.0028293173994383 11.8323265623202385   T   T   T
  6.6677353555526198  1.3279058808108413 13.5897573162018688   T   T   T
  5.3323894838800010  2.6661947419400005  8.0000000000000000   F   F   F
  6.6654868548500010  3.9992921129100010  9.8852843819896918   F   F   F
  5.3447688922203742  2.6653447508923387 11.8283595103154386   T   T   T
  6.6630744702018276  4.0036167571332264 13.5917030261506824   T   T   T
  5.3323894838800010  5.3323894838800010  8.0000000000000000   F   F   F
  6.6654868548500010  6.6654868548500010  9.8852843819896918   F   F   F
  5.3291738766800973  5.3292013933020632 11.8363245928518435   T   T   T
  6.6663913338717311  6.6662576692200322 13.5913198934212449   T   T   T
  2.6672024949323516  2.6662662654857199 14.7006205419454936   T   T   T

fcc100-1x1x4-freeze-2_kpts.12_clean/Au E_tot= -13.86261388 eV
Au
 1.0000000000000000
     2.8987517104700005    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8987517104700005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.0591025586145371
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.4493758552350002  1.4493758552350002 10.0497269914494414   F   F   F
  0.0000000000000000  0.0000000000000000 12.1169801558395065   T   T   T
  1.4493758552350002  1.4493758552350002 14.1968019048596865   T   T   T

fcc100-1x1x4-freeze-2_kpts.12_clean/Ag E_tot= -11.38723968 eV
Ag
 1.0000000000000000
     2.8805270519500006    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8805270519500006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.0210085491588217
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  7.9999999999999991   F   F   F
  1.4402635259750003  1.4402635259750003 10.0368402118251403   F   F   F
  0.0000000000000000  0.0000000000000000 12.0883531465155709   T   T   T
  1.4402635259750003  1.4402635259750003 14.1423768032525405   T   T   T

fcc100-1x1x4-freeze-2_kpts.12_clean/Cu E_tot= -15.08585764 eV
Cu
```

```
 1.0000000000000000
     2.5237696367300004    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.5237696367300004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   21.2752979870721788
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.2618848183650002  1.2618848183650002  9.7845746242844953   F   F   F
  0.0000000000000000  0.0000000000000000 11.6000790539755485   T   T   T
  1.2618848183650002  1.2618848183650002 13.3812534624355717   T   T   T

fcc100-1x1x4-freeze-2_kpts.12_clean/Pt E_tot= -24.79087269 eV
Pt
 1.0000000000000000
     2.7704533654200003    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7704533654200003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   21.7909275272896146
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3852266827100002  1.3852266827100002  9.9590063616495765   F   F   F
  0.0000000000000000  0.0000000000000000 11.9030065873828050   T   T   T
  1.3852266827100002  1.3852266827100002 13.8422650745803892   T   T   T

fcc100-1x1x4-freeze-2_kpts.12_clean/Pd E_tot= -21.00729969 eV
Pd
 1.0000000000000000
     2.7479812319000003    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7479812319000003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   21.7439552525629587
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3739906159500002  1.3739906159500002  9.9431161636498544   F   F   F
  0.0000000000000000  0.0000000000000000 11.8856066366263899   T   T   T
  1.3739906159500002  1.3739906159500002 13.8362334986437023   T   T   T

fcc100-1x1x4-freeze-2_kpts.12_clean/Ni E_tot= -21.25415014 eV
Ni
 1.0000000000000000
     2.4538580817700004    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.4538580817700004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   21.1291656777733685
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.2269290408850002  1.2269290408850002  9.7351396896889817   F   F   F
  0.0000000000000000  0.0000000000000000 11.5140617267014616   T   T   T
  1.2269290408850002  1.2269290408850002 13.2322489426263985   T   T   T

fcc100-1x1x4-freeze-2_kpts.12_clean/Ir E_tot= -34.5932476 eV
Ir
 1.0000000000000000
     2.7150632145500007    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7150632145500007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   21.6751485167430218
   4
Selective dynamics
Cartesian
```

```
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3575316072750003  1.3575316072750003  9.9198396103584514   F   F   F
  0.0000000000000000  0.0000000000000000 11.8576378145328967   T   T   T
  1.3575316072750003  1.3575316072750003 13.7033137722090217   T   T   T

fcc100-1x1x4-freeze-2_kpts.12_clean/Rh E_tot= -28.43295863 eV
Rh
 1.0000000000000000
     2.6776626952800004    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.6776626952800004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   21.5969722517031855
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  7.9999999999999991   F   F   F
  1.3388313476400002  1.3388313476400002  9.8933934495627351   F   F   F
  0.0000000000000000  0.0000000000000000 11.7975396532730770   T   T   T
  1.3388313476400002  1.3388313476400002 13.6489896002686528   T   T   T

fcc100-1x1x4-freeze-2_kpts.12_clean/Os E_tot= -42.60907623 eV
Os
 1.0000000000000000
     2.7084142830800007    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7084142830800007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   21.6612506180246100
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  8.0000000000000000   F   F   F
  1.3542071415400003  1.3542071415400003  9.9151381058283707   F   F   F
  0.0000000647498400 -0.0000000000000000 11.8953353529116548   T   T   T
  1.3542071415314403  1.3542071415400003 13.6848083674392456   T   T   T

fcc100-1x1x4-freeze-2_kpts.12_clean/Ru E_tot= -35.36369316 eV
Ru
 1.0000000000000000
     2.6661947419400005    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.6661947419400005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   21.5730014144722873
   4
Selective dynamics
Cartesian
  0.0000000000000000  0.0000000000000000  7.9999999999999991   F   F   F
  1.3330973709700003  1.3330973709700003  9.8852843819896901   F   F   F
 -0.0000004966756331 -0.0000007246841914 11.8280911438646381   T   T   T
  1.3330977628329219  1.3330978860287690 13.6018919116046728   T   T   T
```

Data for γ_{adh} calculations:

```
Interface: O-a-SiO2(0001)/fcc(111)_2x2/Au E_tot= -258.28340637 eV
 D3-zero damping= -10.4263465 eV, D3-BJ damping= -11.2677251 eV
Si  O Si  O Si  O  H Au
 1.0000000000000000
     5.7975034209400009    0.0000000000000000    0.0000000000000000
    -2.8987517104699987    5.0207852410612297    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.3808530966771428
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.9896011058783145  0.2144519138820970  9.0169746245084816   F   F   F
```

```
 -1.4556949230208058  2.7695472611671716 10.8612336967246357   F   F   F
  2.6817916157075747  3.0604939348830729 11.6081185941916658   F   F   F
  4.0689630393130791  1.6488912642944389  9.5654178022134708   F   F   F
 -0.7325277417681451  4.3923444402091381 10.2987723773365900   F   F   F
  1.2900346052090175  4.0111344900903676  8.2518078419286880   F   F   F
 -0.2278236307478303  2.0064622891632347 11.9218080039603862   F   F   F
  3.0456998983519150 -0.0523678006740076 14.5050718430130097   F   F   F
  1.4266143016520272  2.3486352582438825 12.6701466762358947   F   F   F
 -1.3471476410165109  2.5142447674192137 15.9816098313096742   T   T   T
  3.0076952085237325  2.8201627713954402 16.7483836992599890   T   T   T
  4.0139378835417743  1.1064731643541679 15.1461783547449738   T   T   T
  2.0285516937455728  0.7020542299461070 13.2917821082657603   F   F   F
 -0.9258115637744613  4.0019612827973203 15.3338421791290980   T   T   T
  1.2351244693473293  3.5919589978238933 13.8903255655927040   F   F   F
  0.0837511785999147  2.0816124499554536 16.7197841719867846   T   T   T
  0.0737991663914925  4.9560019170694236 18.9492364476267348   T   T   T
  1.5405944070819531  2.4544436621429071 17.4670658298640227   T   T   T
  4.5681661869369519  2.3949074218180848 20.4815238726996114   T   T   T
  3.9369208363100197  1.0360366744898066 19.7440833161633797   T   T   T
  1.9242476753144675  0.9896744740002825 18.1844951893593958   T   T   T
 -0.9147095399117949  3.8323922547572571 19.6838792949968138   T   T   T
  1.1475085183550209  3.9176020952076089 18.1870666504556127   T   T   T
  0.1767575991156729  1.9616346346796789 21.1939731989613875   T   T   T
  3.3743961396673430  2.8477857318164337 21.5613563121418892   T   T   T
  1.6091618368261216  0.7947340952602039  8.0000000000000000   F   F   F
  1.3744876521683675  1.9300048275022932  8.0158744918591083   F   F   F
  2.3055239184628333  4.4844795339060237  8.0308754104330902   F   F   F
  7.2440299354093467 -1.0049497017498523 23.2001292230904816   T   T   T
  5.5907770096497016 -0.0676104359895171 25.5583875071631255   T   T   T
  5.5718664472252177 -1.6974467833193911 27.9278631097948313   T   T   T
  6.9995913072779876 -0.8521740870458945 30.3680202711813934   T   T   T
  4.2772593756035207 -1.0670921741589865 23.1648963664398693   T   T   T
  2.6831846732961870 -0.0697025252211346 25.5193113318142863   T   T   T
  2.6699859354182673 -1.6892371268969808 27.9257684994522108   T   T   T
  4.1000085985828205 -0.8540610394577746 30.3803738595840898   T   T   T
  5.7701785650268587  1.3998604147591371 23.2200002249551964   T   T   T
  4.1504203568983842  2.4273860576763462 25.5737324869678417   T   T   T
  4.1055333511774146  0.7960595005902334 27.9255848688396711   T   T   T
  5.5481836946095955  1.6571192293067611 30.3281533247574409   T   T   T
  2.8578468531424925  1.3850073810882353 23.1498303851482667   T   T   T
  1.2607482419815415  2.4458203207059328 25.5783268256267426   T   T   T
  1.2188865334332066  0.8071584962348174 27.9327222605567229   T   T   T
  2.6502552710452871  1.6582205474710752 30.3581635764411715   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_2x2/Au E_tot= -210.45703398 eV
 D3-zero damping= -1.7052699 eV, D3-BJ damping= -2.508052 eV
Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     5.7975034209400009    0.0000000000000000    0.0000000000000000
    -2.8987517104699987    5.0207852410612297    0.0000000000000000
     0.0000000000000018    0.0000000000000031   29.5962399724274228
   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.9896011058783145  0.2144519138820970  9.0169746245084816   F   F   F
 -1.4556949230208058  2.7695472611671716 10.8612336967246357   F   F   F
  2.6817916157075747  3.0604939348830729 11.6081185941916623   F   F   F
  4.0689630393130791  1.6488912642944389  9.5654178022134708   F   F   F
 -0.7325277417681451  4.3923444402091381 10.2987723773365900   F   F   F
  1.2900346052090175  4.0111344900903676  8.2518078419286844   F   F   F
 -0.2278236307478303  2.0064622891632347 11.9218080039603862   F   F   F
  3.0456998983519150 -0.0523678006740076 14.5050718430130097   F   F   F
  1.4266143016520272  2.3486352582438825 12.6701466762358947   F   F   F
```

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 -1.3489419197205725  2.5158410263314543 15.9851281092895370   T   T   T
  3.0071882871743862  2.8199717143676302 16.7615572132022805   T   T   T
  4.0106834753518266  1.1085610186427999 15.1515139438926720   T   T   T
  2.0285516937455728  0.7020542299461070 13.2917821082657603   F   F   F
 -0.9267505431033248  4.0044453188510838 15.3400085912386253   T   T   T
  1.2351244693473293  3.5919589978238933 13.8903255655927005   F   F   F
  0.0840475352781916  2.0849653798326275 16.7242153721197901   T   T   T
  0.0805069158922634  4.9707223659071120 18.9794240180983138   T   T   T
  1.5354679135055846  2.4608265583225308 17.4766332078051327   T   T   T
  4.4350209685155200  2.4679863788260672 20.5348327007624682   T   T   T
  3.9316927186482284  1.0593489635144913 19.7755112293500552   T   T   T
  1.9170249688751864  1.0017579948393898 18.2160089985166849   T   T   T
 -0.8719033117170072  3.8670392872191175 19.7725931583593884   T   T   T
  1.1375886711197931  3.9269759463227683 18.1970565604677610   T   T   T
  0.0037889918291354  2.0105239288792500 21.3502882203578466   T   T   T
  3.1913009374879846  2.9997299737719727 21.4610339720909202   T   T   T
  2.3320506054634857  2.5394498604507194 21.4507555561224166   T   T   T
  0.0122823301665650  1.0670391900742877 21.5961505009988528   T   T   T
  1.6091618368261216  0.7947340952602039  8.0000000000000000   F   F   F
  1.3744876521683675  1.9300048275022932  8.0158744918591047   F   F   F
  2.3055239184628333  4.4844795339060237  8.0308754104330866   F   F   F

Oxidized reference: O-a-SiO2(0001)/fcc(111)_2x2/Au E_tot= -198.03609628 eV
 D3-zero damping= -1.645653 eV, D3-BJ damping= -2.4606044 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     5.7975034209400009    0.0000000000000000    0.0000000000000000
    -2.8987517104699987    5.0207852410612297    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.2989605531014377
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.9896011058783145  0.2144519138820970  9.0169746245084816   F   F   F
 -1.4556949230208058  2.7695472611671716 10.8612336967246357   F   F   F
  2.6817916157075747  3.0604939348830729 11.6081185941916623   F   F   F
  4.0689630393130791  1.6488912642944389  9.5654178022134708   F   F   F
 -0.7325277417681451  4.3923444402091381 10.2987723773365900   F   F   F
  1.2900346052090175  4.0111344900903676  8.2518078419286844   F   F   F
 -0.2278236307478303  2.0064622891632347 11.9218080039603862   F   F   F
  3.0456998983519150 -0.0523678006740076 14.5050718430130097   F   F   F
  1.4266143016520272  2.3486352582438825 12.6701466762358947   F   F   F
 -1.3579004881491652  2.5188493988178160 15.9838540605976984   T   T   T
  2.9971178465605415  2.8264879651913088 16.7543443278626931   T   T   T
  4.0086781813212493  1.1063999158713338 15.1587331573894506   T   T   T
  2.0285516937455728  0.7020542299461070 13.2917821082657603   F   F   F
 -0.9282106697372741  3.9986942535656298 15.3323710413431744   T   T   T
  1.2351244693473293  3.5919589978238933 13.8903255655927005   F   F   F
  0.0608995955282895  2.0930461460560568 16.7531955406896600   T   T   T
  0.0418151298913969  4.9493396448240858 18.9500620788819027   T   T   T
  1.5351943602317397  2.4601510168523677 17.4731659299457682   T   T   T
  4.9210451839238756  2.2266122682751464 20.2436265315507704   T   T   T
  3.8628425309344090  1.0881334304145700 19.7351470538251483   T   T   T
  1.9025162501192068  0.9644129822253731 18.1522901393429557   T   T   T
 -0.9463835484459442  3.7759321914685025 19.6549811813246187   T   T   T
  1.1439409981118940  3.9319291431366770 18.1956817771063371   T   T   T
  0.6542105351347268  1.6858971599888726 20.5539830113227033   T   T   T
  5.4619968861916419  2.0940234791740253 21.7894598987737282   T   T   T
  1.6091618368261216  0.7947340952602039  8.0000000000000000   F   F   F
  1.3744876521683675  1.9300048275022932  8.0158744918591047   F   F   F
  2.3055239184628333  4.4844795339060237  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_2x2/Au E_tot= -56.88869091 eV
 D3-zero damping= -7.8509195 eV, D3-BJ damping= -7.8699604 eV
```

```
Au
 1.0000000000000000
     5.7975034209400009    0.0000000000000000    0.0000000000000000
    -2.8987517104699987    5.0207852410612297    0.0000000000000000
     0.0000000000000014    0.0000000000000025   23.2305434744358230
  16
Cartesian
  7.1362531530487789 -0.9008207788154448  7.9795811708354911
  5.6491063300224216 -0.1061954775133738 10.4213099390882267
  5.5939571416268139 -1.7806686018722049 12.7937472493566808
  6.9892358832012036 -0.9153074406845861 15.2370239176391635
  4.2385629708568846 -0.9020906436534462  7.9771383580393449
  2.7513199583242551 -0.1039608190224278 10.4199527906965450
  2.6956419605275412 -1.7798950093595984 12.7944274039940531
  4.0895766459090375 -0.9156095309086716 15.2347593148523526
  5.6888553376733588  1.6093962279638416  7.9804995999269082
  4.2011555449816713  2.4050692599558703 10.4219812222789194
  4.1439431978720354  0.7306726878886437 12.7937724919774301
  5.5418735880345595  1.5939469683443568 15.2328322110602841
  2.7904340395986114  1.6091581030436246  7.9785322999966217
  1.3011580353072618  2.4058850180675848 10.4228420648345192
  1.2457711270847125  0.7285882333599597 12.7915864212110009
  2.6419137551204135  1.5961889500882342 15.2339959347637599

Interface: O-a-SiO2(0001)/fcc(111)_2x2/Ag E_tot= -249.93799094 eV
 D3-zero damping= -8.3902479 eV, D3-BJ damping= -10.5404988 eV
Si  O Si  O Si  O  H Ag
 1.0000000000000000
     5.7610541039000012    0.0000000000000000    0.0000000000000000
    -2.8805270519499988    4.9892192065539964    0.0000000000000000
     0.0000000000000023    0.0000000000000041   38.2674039487523032
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.9708052707369830  0.2131036394212851  9.0169746245084816   F   F   F
 -1.4465428653314458  2.7521349202248735 10.8612336967246357   F   F   F
  2.6649310007602720  3.0412523914751581 11.6081185941916658   F   F   F
  4.0433811787990726  1.6385245674435709  9.5654178022134708   F   F   F
 -0.7279222876680467  4.3647294577889806 10.2987723773365900   F   F   F
  1.2819240657399074  3.9859162017852130  8.2518078419286880   F   F   F
 -0.2263912873504399  1.9938475178045214 11.9218080039603862   F   F   F
  3.0265513661056458 -0.0520385605803217 14.5050718430130097   F   F   F
  1.4176450759010086  2.3338692210510708 12.6701466762358947   F   F   F
 -1.3480765064454934  2.5057945855466164 16.0005432376258412   T   T   T
  2.9740891236198568  2.8144189058231079 16.7710070077404794   T   T   T
  3.9849618276994838  1.1070967643187739 15.1548418265517224   T   T   T
  2.0157980447265311  0.6976403649858635 13.2917821082657603   F   F   F
 -0.9273400968138290  3.9867354775032857 15.3455358695935065   T   T   T
  1.2273591538143542  3.5693760957020113 13.8903255655927040   F   F   F
  0.0768737131156800  2.0715379538740635 16.7433789181465222   T   T   T
  0.0559211604064104  4.9354056013813192 19.0220491801650056   T   T   T
  1.5179263140062516  2.4505246268467804 17.5084582209777508   T   T   T
  4.4620884055229695  2.4165806719137497 20.5794633549451618   T   T   T
  3.9372206074957647  1.0099250994173323 19.8246520609121113   T   T   T
  1.9085811065633198  1.0096892659782273 18.2528353504411811   T   T   T
 -0.9637596445106811  3.8448661681830902 19.7613385892564573   T   T   T
  1.1129547027597777  3.8920028383478487 18.2497817438951984   T   T   T
  0.0961775565409494  2.0681139390016634 21.3651728981385141   T   T   T
  3.2301771495236129  2.7709558996048362 21.6208282493450490   T   T   T
  1.5990449217161975  0.7897375453839228  8.0000000000000000   F   F   F
  1.3658461503763206  1.9178707496521148  8.0158744918591083   F   F   F
  2.2910289253346137  4.4562852915877968  8.0308754104330902   F   F   F
  7.2548040694407971 -1.2983876288710900 23.3288773201770852   T   T   T
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  5.7397589019998962 -0.5084060410035226 25.5445959539439826   T   T   T
  5.7499287016636726 -2.1435851920505966 27.8754866491681810   T   T   T
  7.1934294000198671 -1.3081407308537283 30.2327754931755202   T   T   T
  4.2061948364076640 -1.3312955563245898 22.5900726030002588   T   T   T
  2.9154305474792559 -0.4817808835840735 25.4904435477765503   T   T   T
  2.8823882951384601 -2.1364796775913626 27.8649219952312670   T   T   T
  4.3111327505894161 -1.3100028070368561 30.2674674917579019   T   T   T
  5.7104103097169689  1.0108999216328811 23.2593950623419303   T   T   T
  4.3168007024890800  1.9892790337078285 25.5788802498316841   T   T   T
  4.3125936287563338  0.3413903000564404 27.8973165605360087   T   T   T
  5.7546523409644346  1.1831156135176060 30.2263366935895306   T   T   T
  2.8578340319710711  1.1245327650414429 23.1738290151723589   T   T   T
  1.4328170058428806  2.0300371932453145 25.4753155553304467   T   T   T
  1.4406891052998636  0.3551755352325150 27.8590641498797496   T   T   T
  2.8694918127833859  1.1801233290659423 30.2451254115659012   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_2x2/Ag E_tot= -211.26677456 eV
 D3-zero damping= -1.7204763 eV, D3-BJ damping= -2.5245141 eV
Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     5.7610541039000012    0.0000000000000000    0.0000000000000000
    -2.8805270519499988    4.9892192065539964    0.0000000000000000
     0.0000000000000018    0.0000000000000031   29.6801869137602132
   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.9708052707369830  0.2131036394212851  9.0169746245084816   F   F   F
 -1.4465428653314458  2.7521349202248735 10.8612336967246357   F   F   F
  2.6649310007602720  3.0412523914751581 11.6081185941916623   F   F   F
  4.0433811787990726  1.6385245674435709  9.5654178022134708   F   F   F
 -0.7279222876680467  4.3647294577889806 10.2987723773365900   F   F   F
  1.2819240657399074  3.9859162017852130  8.2518078419286844   F   F   F
 -0.2263912873504399  1.9938475178045214 11.9218080039603862   F   F   F
  3.0265513661056458 -0.0520385605803217 14.5050718430130097   F   F   F
  1.4176450759010086  2.3338692210510708 12.6701466762358947   F   F   F
 -1.3392856166696443  2.5014013641115298 16.0036915558389232   T   T   T
  2.9909773770532522  2.8004887770597624 16.7945639709023489   T   T   T
  3.9877185653392924  1.1067733376917710 15.1566219046512103   T   T   T
  2.0157980447265311  0.6976403649858635 13.2917821082657603   F   F   F
 -0.9248250033055639  3.9852821193462740 15.3519311417868565   T   T   T
  1.2273591538143542  3.5693760957020113 13.8903255655927005   F   F   F
  0.0877733632926506  2.0705999748658734 16.7473411221643964   T   T   T
  0.0793684184310986  4.9387197941642746 19.0380499928765055   T   T   T
  1.5264844023470212  2.4440681433220681 17.5162255856605427   T   T   T
  4.4108093049660377  2.4489126897128988 20.6122397335734604   T   T   T
  3.9103709967216944  1.0507870105493091 19.8406668937067181   T   T   T
  1.9010693982692259  0.9947167047285731 18.2691951784878626   T   T   T
 -0.8684829188157734  3.8421008961894425 19.8406312167150745   T   T   T
  1.1296457923636141  3.9020875608144650 18.2449765695086725   T   T   T
  0.0208953786251514  1.9952771174614417 21.4219503701409657   T   T   T
  3.1740203813436438  2.9697178892251297 21.5533925409438005   T   T   T
  2.3034764551921776  2.5309598789047834 21.5215128860673950   T   T   T
  0.0297339775223937  1.0550381029602838 21.6800842994744976   T   T   T
  1.5990449217161975  0.7897375453839228  8.0000000000000000   F   F   F
  1.3658461503763206  1.9178707496521148  8.0158744918591047   F   F   F
  2.2910289253346137  4.4562852915877968  8.0308754104330866   F   F   F

Oxidized reference: O-a-SiO2(0001)/fcc(111)_2x2/Ag E_tot= -198.83955858 eV
 D3-zero damping= -1.6571209 eV, D3-BJ damping= -2.4704978 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     5.7610541039000012    0.0000000000000000    0.0000000000000000
    -2.8805270519499988    4.9892192065539964    0.0000000000000000
```

```
     0.0000000000000019    0.0000000000000032   30.2989605531014377
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.9708052707369830  0.2131036394212851  9.0169746245084816   F   F   F
 -1.4465428653314458  2.7521349202248735 10.8612336967246357   F   F   F
  2.6649310007602720  3.0412523914751581 11.6081185941916623   F   F   F
  4.0433811787990726  1.6385245674435709  9.5654178022134708   F   F   F
 -0.7279222876680467  4.3647294577889806 10.2987723773365900   F   F   F
  1.2819240657399074  3.9859162017852130  8.2518078419286844   F   F   F
 -0.2263912873504399  1.9938475178045214 11.9218080039603862   F   F   F
  3.0265513661056458 -0.0520385605803217 14.5050718430130097   F   F   F
  1.4176450759010086  2.3338692210510708 12.6701466762358947   F   F   F
 -1.3557067219944134  2.5080648769213814 16.0043250079258570   T   T   T
  2.9670308553552296  2.8095872100763160 16.7817170052459268   T   T   T
  3.9837138386563673  1.1063928152815321 15.1650121448373056   T   T   T
  2.0157980447265311  0.6976403649858635 13.2917821082657603   F   F   F
 -0.9286658768182177  3.9830064283626001 15.3472135831206167   T   T   T
  1.2273591538143542  3.5693760957020113 13.8903255655927005   F   F   F
  0.0553529553113138  2.0829569827172474 16.7822447220266966   T   T   T
  0.0289662354317248  4.9181753819185845 19.0255780135446706   T   T   T
  1.5166729041577500  2.4481007869983653 17.5190684756182513   T   T   T
  4.8779356272472985  2.2121939082209185 20.3448947828575477   T   T   T
  3.8270252199015813  1.0728563661923383 19.8291880580333562   T   T   T
  1.8817988823797698  0.9655607405353225 18.2193998241954986   T   T   T
 -0.9566255764291407  3.7518796081214880 19.7373756931856512   T   T   T
  1.1260646176494478  3.9063708308234806 18.2606086065770050   T   T   T
  0.6454401461136772  1.6783510009099396 20.6732594065109225   T   T   T
  5.4022314254210819  2.0875418529549439 21.8969903259710428   T   T   T
  1.5990449217161975  0.7897375453839228  8.0000000000000000   F   F   F
  1.3658461503763206  1.9178707496521148  8.0158744918591047   F   F   F
  2.2910289253346137  4.4562852915877968  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_2x2/Ag E_tot= -46.54133589 eV
 D3-zero damping= -5.8248367 eV, D3-BJ damping= -7.2172086 eV
Ag
 1.0000000000000000
     5.7610541039000012    0.0000000000000000    0.0000000000000000
    -2.8805270519499988    4.9892192065539964    0.0000000000000000
     0.0000000000000014    0.0000000000000025   23.6773948887576431
  16
Cartesian
  7.1817383744129932 -1.3456540333776745  8.5484930803553230
  5.7465246978454001 -0.5034909488703445 10.9240391431381578
  5.7540960708698607 -2.1500359714528385 13.2588592047586378
  7.1961777609980615 -1.3164318539617743 15.6372287415516542
  4.3016613867637643 -1.3455969713344809  8.5464356755849842
  2.8661093550036356 -0.5027316058188208 10.9236300154004802
  2.8737227903672871 -2.1490391648345426 13.2579401342754188
  4.3153467112169759 -1.3165553407672448 15.6353964825958531
  5.7416645763675049  1.1493825066027576  8.5484500058729136
  4.3061085361935847  1.9914392364648521 10.9245691814198800
  4.3144560051214640  0.3443451425202110 13.2585669636064587
  5.7557831227257781  1.1780943657123710 15.6371303907046730
  2.8615942336093090  1.1481691787005899  8.5491418365792651
  1.4251230725848212  1.9917922000698760 10.9233773691310034
  1.4334999429666822  0.3446367988777193 13.2583628767853927
  2.8747514372786527  1.1781515913925158 15.6371211402643802

Interface: O-a-SiO2(0001)/fcc(111)_2x2/Cu E_tot= -275.45695756 eV
 D3-zero damping= -8.7577968 eV, D3-BJ damping= -11.0278349 eV
Si  O Si  O Si  O  H Cu
 1.0000000000000000
```

```
     5.0475392734600009    0.0000000000000000    0.0000000000000000
    -2.5237696367299991    4.3712972374160097    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.5121006377820621
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.6028667683741604  0.1867104474106613  9.0169746245084816   F   F   F
 -1.2673864525176088  2.4112790550416396 10.8612336967246357   F   F   F
  2.3348754663304621  2.6645889119637172 11.6081185941916658   F   F   F
  3.5426026087380706  1.4355909449108764  9.5654178022134708   F   F   F
 -0.6377680661849743  3.8241514415397448 10.2987723773365900   F   F   F
  1.1231559278423358  3.4922547517148961  8.2518078419286880   F   F   F
 -0.1983524010470477  1.7469066372065702 11.9218080039603862   F   F   F
  2.6517086297142392 -0.0455935100636679 14.5050718430130097   F   F   F
  1.2420676958394576  2.0448161638336280 12.6701466762358947   F   F   F
 -1.3216590680456115  2.2690143314972531 16.3125953409121358   T   T   T
  2.3150918536681777  2.5258166109374249 17.0614194121926523   T   T   T
  3.5845373715387434  1.0882172431341715 15.1966095960609273   T   T   T
  1.7661385598224295  0.6112366031475546 13.2917821082657603   F   F   F
 -0.8779897675464159  3.6680523369942843 15.6035391428996508   T   T   T
  1.0753489586783649  3.1273037364132263 13.8903255655927040   F   F   F
 -0.2057920761981555  1.8130340105059242 17.3993300039695562   T   T   T
 -0.0793588564406789  4.4395461364866602 19.9962921165125849   T   T   T
  1.1454924973892175  2.3010182343286814 18.1591679627444229   T   T   T
  3.8618485340186353  2.1778882194734757 21.8062368455604201   T   T   T
  3.3591071605675404  0.7784906236392024 21.1358711796233862   T   T   T
  1.5197517264245037  1.1684967721651756 19.2521048217588060   T   T   T
 -1.0652150757409096  3.3296020152118331 20.6620981105165420   T   T   T
  0.8957348014824903  3.7207692217559143 18.9110796297111570   T   T   T
  0.2141111855753508  1.9532234766060887 22.6095667880786060   T   T   T
  2.7497922935574466  2.6471145962100722 22.9393088414535917   T   T   T
  1.4010009100461971  0.6919274153930846  8.0000000000000000   F   F   F
  1.1966841416853842  1.6803397009821337  8.0158744918591083   F   F   F
  2.0072817003108723  3.9043679537403611  8.0308754104330902   F   F   F
  6.3056296568889447 -0.9302862760390022 24.4283188603369403   T   T   T
  4.9823133776146253 -0.2494511296029635 26.3709889925696572   T   T   T
  4.9991802618023682 -1.6912793695682029 28.4303375378791650   T   T   T
  6.2604572601069703 -0.9560453203795470 30.4973466488613028   T   T   T
  3.6759690212379357 -1.0008519957817041 23.9899829894640888   T   T   T
  2.5082495302844761 -0.2425396780292927 26.3418729634662050   T   T   T
  2.4829798843331248 -1.6858437912845123 28.4317555666927326   T   T   T
  3.7355635533768545 -0.9584632561520775 30.5108124600181974   T   T   T
  5.0103518413249839  1.1418743200153361 24.3656797320650576   T   T   T
  3.7522674040735784  1.9336188834447268 26.4139485134216514   T   T   T
  3.7374950113638485  0.4878147260215220 28.4459667639445009   T   T   T
  4.9982493785562978  1.2264666904927073 30.4916095375106089   T   T   T
  2.5097033808891362  1.1803890620851103 24.3438542103966817   T   T   T
  1.2237790330963416  1.9565647021544339 26.3608464032694414   T   T   T
  1.2188628201847562  0.4928402214909474 28.4161058344126474   T   T   T
  2.4719670244788317  1.2252287384553373 30.5000294025746292   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_2x2/Cu E_tot= -221.09750805 eV
 D3-zero damping= -2.1846112 eV, D3-BJ damping= -3.1100996 eV
Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     5.0475392734600009    0.0000000000000000    0.0000000000000000
    -2.5237696367299991    4.3712972374160097    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.7542840754157361
   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.6028667683741604  0.1867104474106613  9.0169746245084816   F   F   F
 -1.2673864525176088  2.4112790550416396 10.8612336967246357   F   F   F
```

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  2.3348754663304621  2.6645889119637172 11.6081185941916623   F   F   F
  3.5426026087380706  1.4355909449108764  9.5654178022134708   F   F   F
 -0.6377680661849743  3.8241514415397448 10.2987723773365900   F   F   F
  1.1231559278423358  3.4922547517148961  8.2518078419286844   F   F   F
 -0.1983524010470477  1.7469066372065702 11.9218080039603862   F   F   F
  2.6517086297142392 -0.0455935100636679 14.5050718430130097   F   F   F
  1.2420676958394576  2.0448161638336280 12.6701466762358947   F   F   F
 -1.3562828735725780  2.2757798285516002 16.2987952043764786   T   T   T
  2.2321989153739930  2.5037143381256604 16.9715738879991562   T   T   T
  3.6004103362915210  1.0820080929669971 15.1897868425513565   T   T   T
  1.7661385598224295  0.6112366031475546 13.2917821082657603   F   F   F
 -0.8815592847618124  3.6713973868067575 15.6060446707272433   T   T   T
  1.0753489586783649  3.1273037364132263 13.8903255655927005   F   F   F
 -0.2942873673263083  1.8375226847496637 17.4507882493989932   T   T   T
  0.1559429609556248  4.4735689437661428 19.9281834236993056   T   T   T
  1.1562420874049573  2.1151584802478078 18.1283894531145577   T   T   T
  3.8668273090055889  2.3458793095786166 21.7467549353935219   T   T   T
  3.5925573241525570  1.3140729282911898 20.5097437684042987   T   T   T
  1.5893142418526447  0.7467263272454497 18.9008002660758976   T   T   T
 -0.5766744049822136  3.7537071942395879 21.1890254178981579   T   T   T
  1.0750417795182798  3.3745940913908283 19.1603509469052256   T   T   T
  0.0021635014498414  1.6659498865025164 22.6875628457854468   T   T   T
  2.5389324916514506  2.8168869904110374 22.5664950872310222   T   T   T
  1.6988323638658178  2.2980571508606831 22.6433817503163795   T   T   T
 -0.0173800649955936  0.6864017171580346 22.7528424952255364   T   T   T
  1.4010009100461971  0.6919274153930846  8.0000000000000000   F   F   F
  1.1966841416853842  1.6803397009821337  8.0158744918591047   F   F   F
  2.0072817003108723  3.9043679537403611  8.0308754104330866   F   F   F

Oxidized reference: O-a-SiO2(0001)/fcc(111)_2x2/Cu E_tot= -208.49395884 eV
 D3-zero damping= -2.0717249 eV, D3-BJ damping= -2.9864571 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     5.0475392734600009    0.0000000000000000    0.0000000000000000
    -2.5237696367299991    4.3712972374160097    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.2989605531014377
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.6028667683741604  0.1867104474106613  9.0169746245084816   F   F   F
 -1.2673864525176088  2.4112790550416396 10.8612336967246357   F   F   F
  2.3348754663304621  2.6645889119637172 11.6081185941916623   F   F   F
  3.5426026087380706  1.4355909449108764  9.5654178022134708   F   F   F
 -0.6377680661849743  3.8241514415397448 10.2987723773365900   F   F   F
  1.1231559278423358  3.4922547517148961  8.2518078419286844   F   F   F
 -0.1983524010470477  1.7469066372065702 11.9218080039603862   F   F   F
  2.6517086297142392 -0.0455935100636679 14.5050718430130097   F   F   F
  1.2420676958394576  2.0448161638336280 12.6701466762358947   F   F   F
 -1.1726595173915924  2.2237128078294375 16.3189765081503957   T   T   T
  2.6291703949059206  2.4559255948748895 17.3219259686778067   T   T   T
  3.5754689633526300  1.0899632950893392 15.1968042328784065   T   T   T
  1.7661385598224295  0.6112366031475546 13.2917821082657603   F   F   F
 -0.8581242816949924  3.6580760769282756 15.6156335625223495   T   T   T
  1.0753489586783649  3.1273037364132263 13.8903255655927005   F   F   F
  0.1010587373566056  1.7092627597614145 17.1838115038017314   T   T   T
 -0.0640193032818560  4.3312599895399382 19.9994407311916724   T   T   T
  1.2808426538691224  2.2149032904668018 18.1736543517798772   T   T   T
  4.2797483423051217  1.9009683172871505 21.6490699364083561   T   T   T
  3.4151868811264303  0.6567609710812762 21.1127851671516140   T   T   T
  1.4884288168407096  1.0739223421758619 19.3194455346708729   T   T   T
 -1.0124543278967983  3.1802557264397207 20.6727355125918422   T   T   T
  0.8731068543759617  3.6348120621367133 18.8621938608102404   T   T   T
  0.7544536037097782  1.6543570219067234 22.2201275026220983   T   T   T
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  4.5988327600148544  2.0940743195291867 23.2422238443276328   T   T   T
  1.4010009100461971  0.6919274153930846  8.0000000000000000   F   F   F
  1.1966841416853842  1.6803397009821337  8.0158744918591047   F   F   F
  2.0072817003108723  3.9043679537403611  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_2x2/Cu E_tot= -61.73568727 eV
 D3-zero damping= -5.7898521 eV, D3-BJ damping= -7.0976399 eV
Cu
 1.0000000000000000
     5.0475392734600009    0.0000000000000000    0.0000000000000000
    -2.5237696367299991    4.3712972374160097    0.0000000000000000
     0.0000000000000014    0.0000000000000024   22.5208294705541086
  16
Cartesian
  6.2669753259974303 -0.9802908151026788  8.3078134146821156
  5.0043285750733215 -0.2469745740159384 10.3806602407139295
  5.0038431273726260 -1.6975894538484873 12.4320576320316594
  6.2643496130699940 -0.9645457474195802 14.5048104348648543
  3.7434044166769436 -0.9799871851811184  8.3106142013126494
  2.4805524858580656 -0.2463488564210304 10.3805511263891947
  2.4800420145084368 -1.6975567896522001 12.4319609981556081
  3.7404685420253818 -0.9644532406710993 14.5023737736755827
  5.0051198343108858  1.2055645392690817  8.3081574686785693
  3.7425386629442992  1.9396207643888015 10.3801699376448830
  3.7417496744820498  0.4881149335113513 12.4316810901841119
  5.0022708073631259  1.2211360541675329 14.5041235718524302
  2.4817450035402007  1.2053911332878149  8.3083311772605484
  1.2186931326135859  1.9387795573486721 10.3796777393789590
  1.2181642984238630  0.4878985649057550 12.4328271096745997
  2.4787734188606199  1.2212774461375500 14.5039182923359196

Interface: O-a-SiO2(0001)/fcc(111)_2x2/Pt E_tot= -309.07900926 eV
 D3-zero damping= -11.5762643 eV, D3-BJ damping= -12.7522351 eV
Si  O Si  O Si  O  H Pt
 1.0000000000000000
     5.5409067308400006    0.0000000000000000    0.0000000000000000
    -2.7704533654199985    4.7985659889076260    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.6792501838884704
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.8572817793011347  0.2049603021843787  9.0169746245084816   F   F   F
 -1.3912660694399051  2.6469674869622617 10.8612336967246357   F   F   F
  2.5630958940900586  2.9250369016149853 11.6081185941916658   F   F   F
  3.8888713046095078  1.5759115676849356  9.5654178022134708   F   F   F
 -0.7001061664284518  4.1979398899563565 10.2987723773365900   F   F   F
  1.2329378541117286  3.8336022388827846  8.2518078419286880   F   F   F
 -0.2177401887328913  1.9176565490320319 11.9218080039603862   F   F   F
  2.9108976470703980 -0.0500500091445998 14.5050718430130097   F   F   F
  1.3634725523033258  2.2446849903853381 12.6701466762358947   F   F   F
 -1.2889132719845908  2.4108310494381961 16.1110022543698221   T   T   T
  2.8692492655313098  2.6722513717651126 16.9586562540528369   T   T   T
  3.8608619075280362  1.0929150089708943 15.1755249546722482   T   T   T
  1.9387682796587782  0.6709814079751512 13.2917821082657603   F   F   F
 -0.9092040831414212  3.8683183817556279 15.4255812992410437   T   T   T
  1.1804580331790768  3.4329793952440149 13.8903255655927040   F   F   F
  0.0846518406566570  1.9748296709087920 16.9109111949885005   T   T   T
  0.0466112885702966  4.6922326708575470 19.3731288804020458   T   T   T
  1.4675514544246027  2.3171091485588344 17.7491092957433843   T   T   T
  4.3797713347068328  2.2256966952169153 21.0334347393204695   T   T   T
  3.7076266251195111  0.9464227624564572 20.2615623019461069   T   T   T
  1.8069907340357743  0.9026172304394696 18.5399899667362966   T   T   T
 -0.8909698297226627  3.5874470501190681 20.1532489802390380   T   T   T
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  1.1049078109049937  3.7199880895219675 18.5521347293377303   T   T   T
  0.2063855349630216  1.7121898353315186 21.7572118908472234   T   T   T
  3.2510261405579777  2.7696780769870810 22.1559899187558500   T   T   T
  1.5379405591165740  0.7595592754201972  8.0000000000000000   F   F   F
  1.3136530210311361  1.8445830839246389  8.0158744918591083   F   F   F
  2.2034817524699370  4.2859970972997328  8.0308754104330902   F   F   F
  6.9750227550700732 -0.8977236709545661 23.7575931276436911   T   T   T
  5.4166904686121926  0.0288057624616367 26.0846423306654280   T   T   T
  5.3396000679327340 -1.5577428197968555 28.3501449893732413   T   T   T
  6.6832259965456702 -0.7484066573359740 30.6478154708705439   T   T   T
  4.1708418311690618 -0.8815927413412133 23.8594502155852624   T   T   T
  2.6177823575747898  0.0192845509941267 25.9904715218914895   T   T   T
  2.5671846976022912 -1.5572783791099074 28.3431211877693450   T   T   T
  3.9093460682467791 -0.7501524300085395 30.6348516075627941   T   T   T
  5.6188420794352618  1.4853252785688758 23.7698194400878045   T   T   T
  4.0249349755407184  2.4093383207830721 26.1098120090018959   T   T   T
  3.9512335854168645  0.8407752335728190 28.3373389481029179   T   T   T
  5.2991255991630082  1.6423347791818903 30.6837789378479187   T   T   T
  2.8174463973113029  1.4661045488213837 23.7616800456031072   T   T   T
  1.2534425880867057  2.4053012122642006 26.1079331680633402   T   T   T
  1.1846767275227266  0.8400808843685302 28.3333677871610874   T   T   T
  2.5211636564507587  1.6403614566608784 30.6586695596627408   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_2x2/Pt E_tot= -215.65784927 eV
 D3-zero damping= -1.8230208 eV, D3-BJ damping= -2.6414642 eV
Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     5.5409067308400006    0.0000000000000000    0.0000000000000000
    -2.7704533654199985    4.7985659889076260    0.0000000000000000
     0.0000000000000018    0.0000000000000032   30.1387437364994391
   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.8572817793011347  0.2049603021843787  9.0169746245084816   F   F   F
 -1.3912660694399051  2.6469674869622617 10.8612336967246357   F   F   F
  2.5630958940900586  2.9250369016149853 11.6081185941916623   F   F   F
  3.8888713046095078  1.5759115676849356  9.5654178022134708   F   F   F
 -0.7001061664284518  4.1979398899563565 10.2987723773365900   F   F   F
  1.2329378541117286  3.8336022388827846  8.2518078419286844   F   F   F
 -0.2177401887328913  1.9176565490320319 11.9218080039603862   F   F   F
  2.9108976470703980 -0.0500500091445998 14.5050718430130097   F   F   F
  1.3634725523033258  2.2446849903853381 12.6701466762358947   F   F   F
 -1.3057039139783615  2.4213698679693048 16.1146498839957637   T   T   T
  2.8451928009256169  2.6976891231897246 16.9495863362849555   T   T   T
  3.8523066657336376  1.0963194760705999 15.1845540394988188   T   T   T
  1.9387682796587782  0.6709814079751512 13.2917821082657603   F   F   F
 -0.9125720518160436  3.8718980773359637 15.4243865602715466   T   T   T
  1.1804580331790768  3.4329793952440149 13.8903255655927005   F   F   F
  0.0625248694480830  1.9883630387882179 16.9277362399393638   T   T   T
  0.0603729719779476  4.7465633002389813 19.3942015484437569   T   T   T
  1.4484140319650447  2.3442568010279170 17.7539710245059013   T   T   T
  4.2453437778385270  2.3440452441287269 21.0775785871760064   T   T   T
  3.7663270697689821  1.0045965145316964 20.2365746416946912   T   T   T
  1.8093760714531388  0.9454671813483695 18.5595325296697951   T   T   T
 -0.8746938239860859  3.7098751724378793 20.2573192168004077   T   T   T
  1.0803605261886815  3.7390879745948258 18.5670843578945295   T   T   T
  0.1021441932581884  1.9056179518653387 21.8554042072290358   T   T   T
  3.0463845270882985  2.8088926783226684 22.0881522813600135   T   T   T
  2.1337002150476314  2.4694442439881072 21.9820344595014916   T   T   T
  0.1183585113635235  0.9725752918020700 22.1402415663831498   T   T   T
  1.5379405591165740  0.7595592754201972  8.0000000000000000   F   F   F
  1.3136530210311361  1.8445830839246389  8.0158744918591047   F   F   F
  2.2034817524699370  4.2859970972997328  8.0308754104330866   F   F   F
```

```
Oxidized reference: O-a-SiO2(0001)/fcc(111)_2x2/Pt E_tot= -203.18651373 eV
 D3-zero damping= -1.7540655 eV, D3-BJ damping= -2.5783924 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     5.5409067308400006    0.0000000000000000    0.0000000000000000
    -2.7704533654199985    4.7985659889076260    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.2989605531014377
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.8572817793011347  0.2049603021843787  9.0169746245084816   F   F   F
 -1.3912660694399051  2.6469674869622617 10.8612336967246357   F   F   F
  2.5630958940900586  2.9250369016149853 11.6081185941916623   F   F   F
  3.8888713046095078  1.5759115676849356  9.5654178022134708   F   F   F
 -0.7001061664284518  4.1979398899563565 10.2987723773365900   F   F   F
  1.2329378541117286  3.8336022388827846  8.2518078419286844   F   F   F
 -0.2177401887328913  1.9176565490320319 11.9218080039603862   F   F   F
  2.9108976470703980 -0.0500500091445998 14.5050718430130097   F   F   F
  1.3634725523033258  2.2446849903853381 12.6701466762358947   F   F   F
 -1.3055023638047996  2.4214448717597055 16.1136023262102448   T   T   T
  2.8498576564045357  2.6955589869363115 16.9593592615546385   T   T   T
  3.8502083939908252  1.0949301961896352 15.1897165010612625   T   T   T
  1.9387682796587782  0.6709814079751512 13.2917821082657603   F   F   F
 -0.9144626372472698  3.8722616266083381 15.4255359614275900   T   T   T
  1.1804580331790768  3.4329793952440149 13.8903255655927005   F   F   F
  0.0634054616273918  1.9891809427528797 16.9266631675401236   T   T   T
  0.0130942502216132  4.7203316476539108 19.3885818423794305   T   T   T
  1.4495413377585424  2.3486395895117291 17.7537022092296120   T   T   T
  4.7090754580243743  2.1140271207804853 20.8219843083815874   T   T   T
  3.6967676123956106  0.9816200904775895 20.2598222381409627   T   T   T
  1.7843253552531873  0.9375863776509904 18.5551358189052991   T   T   T
 -0.9572836478997246  3.6037613280860619 20.1452755055517514   T   T   T
  1.0678241809356699  3.7495693367212839 18.5548424762787647   T   T   T
  0.7007970769168028  1.6435756680366731 21.2071201523187334   T   T   T
  5.1791336643268151  2.0225776956024526 22.3909722519096093   T   T   T
  1.5379405591165740  0.7595592754201972  8.0000000000000000   F   F   F
  1.3136530210311361  1.8445830839246389  8.0158744918591047   F   F   F
  2.2034817524699370  4.2859970972997328  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_2x2/Pt E_tot= -101.65816216 eV
 D3-zero damping= -8.8416925 eV, D3-BJ damping= -9.2321093 eV
Pt
 1.0000000000000000
     5.5409067308400006    0.0000000000000000    0.0000000000000000
    -2.7704533654199985    4.7985659889076260    0.0000000000000000
     0.0000000000000014    0.0000000000000024   22.9261858102042275
  16
Cartesian
  6.8309713953146209 -0.8006057754104720  8.0268850665684521
  5.4251035861260197 -0.0054638293023725 10.3281316239012213
  5.3926613913337471 -1.6022175394650167 12.5861423870268698
  6.7499710198101477 -0.7945076737131038 14.8860987078863793
  4.0605680951817167 -0.8005739197051500  8.0269555250323084
  2.6547930388085406 -0.0054227402179966 10.3282668576069092
  2.6222299857567251 -1.6020058899646932 12.5862365031846135
  3.9795916543120891 -0.7944965631439842 14.8862007428033625
  5.4457988058985300  1.5986481797717995  8.0264644187056646
  4.0399081061457816  2.3940312023294976 10.3278597721904308
  4.0075838916306310  0.7971239445038707 12.5862350794487625
  5.3650119679439880  1.6050479806884850 14.8863501416234048
  2.6752997438543131  1.5986255274168939  8.0270694347625167
  1.2694464617894481  2.3939925322092850 10.3280134188983492
```

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  1.2369879849851320  0.7973164696963854 12.5861882643250560
  2.5946286072494380  1.6053222834431202 14.8859019769687997

Interface: O-a-SiO2(0001)/fcc(111)_2x2/Pd E_tot= -294.17629909 eV
 D3-zero damping= -9.3768866 eV, D3-BJ damping= -11.5290048 eV
Si  O Si  O Si  O  H Pd
 1.0000000000000000
     5.4959624638000006    0.0000000000000000    0.0000000000000000
    -2.7479812318999985    4.7596431118965139    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.5228487912856394
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.8341053496054900  0.2032977962081091  9.0169746245084816   F   F   F
 -1.3799810150641352  2.6254969913630339 10.8612336967246357   F   F   F
  2.5423057108386526  2.9013108860016326 11.6081185941916658   F   F   F
  3.8573272850313138  1.5631287879396571  9.5654178022134708   F   F   F
 -0.6944273560768578  4.1638889050549253 10.2987723773365900   F   F   F
  1.2229370562548547  3.8025065263723210  8.2518078419286880   F   F   F
 -0.2159740205472254  1.9021017540828602 11.9218080039603862   F   F   F
  2.8872863199841889 -0.0496440357027750 14.5050718430130097   F   F   F
  1.3524129410394594  2.2264775513272066 12.6701466762358947   F   F   F
 -1.2991533275458322  2.4032676821172800 16.1309340188566459   T   T   T
  2.8146657125455374  2.6715902838116383 16.9705044552410591   T   T   T
  3.8277371934495710  1.0940304569547719 15.1816862806851063   T   T   T
  1.9230422399467801  0.6655388389076984 13.2917821082657603   F   F   F
 -0.9112763881346687  3.8509482001480908 15.4380243770724999   T   T   T
  1.1708829178324462  3.4051332772388347 13.8903255655927040   F   F   F
  0.0561609468088883  1.9659733295828858 16.9518550303910871   T   T   T
  0.0146880780191004  4.6633098390859233 19.4343218849409070   T   T   T
  1.4324893143981201  2.3162885255752488 17.7884400115584498   T   T   T
  4.3106591264723919  2.2272161096559686 21.0991086493326314   T   T   T
  3.6554637164922616  0.9196688430889765 20.3575444525093552   T   T   T
  1.7804700638490580  0.9192598432089938 18.5897089885456559   T   T   T
 -0.9616179008068604  3.5747960913648935 20.1860819332375776   T   T   T
  1.0744066040770821  3.7035620412882868 18.6084557428053046   T   T   T
  0.2307392580000952  1.7942588357819365 21.7820271451259160   T   T   T
  3.1883332998075731  2.7212018907879836 22.2466016535589972   T   T   T
  1.5254657757393588  0.7533982197364427  8.0000000000000000   F   F   F
  1.3029975137210219  1.8296210138648872  8.0158744918591083   F   F   F
  2.1856085275427661  4.2512318490414387  8.0308754104330902   F   F   F
  7.0209704756176947 -1.0176002805455364 23.7596538517436962   T   T   T
  5.5678065527607696 -0.1812136114790458 25.9810787366869000   T   T   T
  5.5614991121206696 -1.7687809349356136 28.2547453730738809   T   T   T
  6.9376879342966173 -0.9752322519943597 30.5155022274536094   T   T   T
  4.2364649491700392 -1.0391728713570934 23.6876156606190733   T   T   T
  2.8236540170699493 -0.1980174461863163 25.9270899192441213   T   T   T
  2.8183826661493172 -1.7657589547360120 28.2361120907550998   T   T   T
  4.1850262351883645 -0.9770306540516693 30.5240595366660692   T   T   T
  5.6408917899737929  1.3172197654649591 23.7326926983040174   T   T   T
  4.2010019469771613  2.1833349485068072 26.0285472452874664   T   T   T
  4.1871985504750269  0.6008294585256447 28.2318786505577748   T   T   T
  5.5632484814182570  1.3997826375080289 30.5196104891266309   T   T   T
  2.8843515470436287  1.2975543886597773 23.7466196014853317   T   T   T
  1.4581312618709064  2.1917007111860913 26.0088339214210649   T   T   T
  1.4448420136314057  0.6044117838548118 28.2210016466110503   T   T   T
  2.8116544606012019  1.3941709244578455 30.5204823790175830   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_2x2/Pd E_tot= -216.4245057 eV
 D3-zero damping= -1.8465129 eV, D3-BJ damping= -2.6698285 eV
Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     5.4959624638000006    0.0000000000000000    0.0000000000000000
```

```
    -2.7479812318999985    4.7596431118965139    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.2520609100293818
   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.8341053496054900  0.2032977962081091  9.0169746245084816   F   F   F
 -1.3799810150641352  2.6254969913630339 10.8612336967246357   F   F   F
  2.5423057108386526  2.9013108860016326 11.6081185941916623   F   F   F
  3.8573272850313138  1.5631287879396571  9.5654178022134708   F   F   F
 -0.6944273560768578  4.1638889050549253 10.2987723773365900   F   F   F
  1.2229370562548547  3.8025065263723210  8.2518078419286844   F   F   F
 -0.2159740205472254  1.9021017540828602 11.9218080039603862   F   F   F
  2.8872863199841889 -0.0496440357027750 14.5050718430130097   F   F   F
  1.3524129410394594  2.2264775513272066 12.6701466762358947   F   F   F
 -1.2886840868935370  2.4016514264900670 16.1349439699797266   T   T   T
  2.8310551964481894  2.6710289842039705 16.9888256207395543   T   T   T
  3.8280226113150095  1.0954716309596706 15.1849629045102539   T   T   T
  1.9230422399467801  0.6655388389076984 13.2917821082657603   F   F   F
 -0.9059288276476328  3.8513595665517624 15.4443670706455283   T   T   T
  1.1708829178324462  3.4051332772388347 13.8903255655927005   F   F   F
  0.0745270741913621  1.9639305686104287 16.9474903034696034   T   T   T
  0.0601848902925383  4.6995864526332998 19.4627001811457383   T   T   T
  1.4416791307630774  2.3176279835507798 17.7981369509010889   T   T   T
  4.2131436175203945  2.3146456983755352 21.1672070452288459   T   T   T
  3.7440992665249322  0.9837656873470182 20.3142561329964515   T   T   T
  1.7919129752839376  0.9306941228155639 18.6207098803106135   T   T   T
 -0.8717039006311836  3.6728706470740273 20.3357955189666448   T   T   T
  1.0710030611077332  3.7009508675742877 18.6217472069929961   T   T   T
  0.1153788776215551  1.8834476050121420 21.9489955235734264   T   T   T
  3.0171194135119066  2.7687091143956790 22.1841219061433144   T   T   T
  2.0972303242984784  2.4505824424825593 22.0655098484414154   T   T   T
  0.1318867538743163  0.9564579265482949 22.2531929025744830   T   T   T
  1.5254657757393588  0.7533982197364427  8.0000000000000000   F   F   F
  1.3029975137210219  1.8296210138648872  8.0158744918591047   F   F   F
  2.1856085275427661  4.2512318490414387  8.0308754104330866   F   F   F

Oxidized reference: O-a-SiO2(0001)/fcc(111)_2x2/Pd E_tot= -203.94781294 eV
 D3-zero damping= -1.7770531 eV, D3-BJ damping= -2.6056956 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     5.4959624638000006    0.0000000000000000    0.0000000000000000
    -2.7479812318999985    4.7596431118965139    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.2989605531014377
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.8341053496054900  0.2032977962081091  9.0169746245084816   F   F   F
 -1.3799810150641352  2.6254969913630339 10.8612336967246357   F   F   F
  2.5423057108386526  2.9013108860016326 11.6081185941916623   F   F   F
  3.8573272850313138  1.5631287879396571  9.5654178022134708   F   F   F
 -0.6944273560768578  4.1638889050549253 10.2987723773365900   F   F   F
  1.2229370562548547  3.8025065263723210  8.2518078419286844   F   F   F
 -0.2159740205472254  1.9021017540828602 11.9218080039603862   F   F   F
  2.8872863199841889 -0.0496440357027750 14.5050718430130097   F   F   F
  1.3524129410394594  2.2264775513272066 12.6701466762358947   F   F   F
 -1.2899635254071189  2.4007087632818647 16.1334027916359162   T   T   T
  2.8291581879533210  2.6675533219494501 16.9879873528474938   T   T   T
  3.8267582647038316  1.0926723772800693 15.1896509108615199   T   T   T
  1.9230422399467801  0.6655388389076984 13.2917821082657603   F   F   F
 -0.9077177878452349  3.8491797319677272 15.4431325134897275   T   T   T
  1.1708829178324462  3.4051332772388347 13.8903255655927005   F   F   F
  0.0670450508674136  1.9628976579634467 16.9573449889197789   T   T   T
  0.0193095898747291  4.6726194209506851 19.4545671526553861   T   T   T
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  1.4420499031809821  2.3215400551702348 17.7959993875217855   T   T   T
  4.6827547830890905  2.0877981667374468 20.9122980147440138   T   T   T
  3.6813105829356374  0.9519064949139160 20.3433441664546955   T   T   T
  1.7740698058760045  0.9253185415706597 18.6159473313387984   T   T   T
 -0.9521095785701499  3.5638326937212117 20.2138041308981151   T   T   T
  1.0666551005454958  3.7127360491248349 18.6075313237329425   T   T   T
  0.7213861243239057  1.6389983514103690 21.3128282626809309   T   T   T
  5.1411386838833666  2.0127232850955399 22.4853909140188506   T   T   T
  1.5254657757393588  0.7533982197364427  8.0000000000000000   F   F   F
  1.3029975137210219  1.8296210138648872  8.0158744918591047   F   F   F
  2.1856085275427661  4.2512318490414387  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_2x2/Pd E_tot= -85.79476816 eV
 D3-zero damping= -6.6597588 eV, D3-BJ damping= -7.9824282 eV
Pd
 1.0000000000000000
     5.4959624638000006    0.0000000000000000    0.0000000000000000
    -2.7479812318999985    4.7596431118965139    0.0000000000000000
     0.0000000000000014    0.0000000000000024   22.8364438760469959
  16
Cartesian
  6.9593192434903370 -1.0117206974963178  8.0289009960199369
  5.5840475604781803 -0.2109966662120503 10.3086637794084695
  5.5818569947744008 -1.7857286249199391 12.5535738049170540
  6.9540907442569395 -0.9852492059187401 14.8320756574400949
  4.2116004955434292 -1.0114545250574454  8.0278099185677494
  2.8362607533537085 -0.2108637775240321 10.3084751439687672
  2.8339284734795056 -1.7850685574269289 12.5534994697086759
  4.2062515302340753 -0.9854357211405819 14.8336623983024598
  5.5851492214972041  1.3686543424891189  8.0286232790686540
  4.2101976998554766  2.1685847546106394 10.3087612758873135
  4.2081366373029132  0.5941372417456265 12.5538034489408918
  5.5804038772992666  1.3945803781796118 14.8322813851544026
  2.8370403143839167  1.3688613980933941  8.0284398204380079
  1.4621453648584273  2.1689901840663075 10.3088883222089951
  1.4599920663349635  0.5944418871960836 12.5534563441142026
  2.8323925493010012  1.3944651350613328 14.8327574867808529

Interface: O-a-SiO2(0001)/fcc(111)_2x2/Ni E_tot= -300.9863746 eV
 D3-zero damping= -7.5479778 eV, D3-BJ damping= -9.6564674 eV
Si  O Si  O Si  O  H Ni
 1.0000000000000000
     4.9077161635400008    0.0000000000000000    0.0000000000000000
    -2.4538580817699986    4.2502068721891453    0.0000000000000000
     0.0000000000000023    0.0000000000000040   37.9724841506789446
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.5307641245819466  0.1815383360119881  9.0169746245084816   F   F   F
 -1.2322782729352804  2.3444836289745989 10.8612336967246357   F   F   F
  2.2701965146094101  2.5907764880984683 11.6081185941916658   F   F   F
  3.4444681144570746  1.3958232918792568  9.5654178022134708   F   F   F
 -0.6201010982644807  3.7182176947390766 10.2987723773365900   F   F   F
  1.0920431130135873  3.3955149556354178  8.2518078419286880   F   F   F
 -0.1928577930664174  1.6985151526591546 11.9218080039603862   F   F   F
  2.5782530056722708 -0.0443305131806539 14.5050718430130097   F   F   F
  1.2076608772780650  1.9881722152178671 12.6701466762358947   F   F   F
 -1.3867501951219507  2.2437484381568820 16.3242800085656299   T   T   T
  2.0317545858938990  2.4617324571608949 16.9272381766628186   T   T   T
  3.5321865701863984  1.0846781279573139 15.1811241147391289   T   T   T
  1.7172143271210711  0.5943045897210512 13.2917821082657603   F   F   F
 -0.8833398951562379  3.6320954695003564 15.6469784810895689   T   T   T
  1.0455604563001411  3.0406735369437734 13.8903255655927040   F   F   F
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 -0.4268091686627560  1.8182077371950598 17.5602148833103016   T   T   T
 -0.1924741422666145  4.0727534956048732 20.0175016536386039   T   T   T
  1.0519293891329677  2.1008512449912855 18.1714530077788901   T   T   T
  3.5986876334226898  1.9370437720850826 21.8321968319429622   T   T   T
  2.8324369499250062  0.6055536571954080 21.3133414407031587   T   T   T
  1.4837533886196015  0.7686503970267937 18.9690659332677178   T   T   T
 -1.2309235537591190  2.9499184160108043 20.5684688631420300   T   T   T
  1.0217875343610299  3.3513127021453397 19.2110899095903243   T   T   T
  0.1203173230001165  1.5779863001539081 22.4981309896049524   T   T   T
  2.6809236230275726  2.6543425141593473 23.0539890366449711   T   T   T
  1.3621914439617202  0.6727601662014105  7.9999999999999991   F   F   F
  1.1635345039674199  1.6337922032838519  8.0158744918591047   F   F   F
  1.9516775029748146  3.7962121098751287  8.0308754104330866   F   F   F
  6.3053836937883823 -0.8135657845194284 24.4130075692329775   T   T   T
  5.0452929027801030 -0.1258041750003772 26.3893492910932608   T   T   T
  5.0466259266041709 -1.5537992718558618 28.4165110794259057   T   T   T
  6.2692609908184771 -0.8501698103735779 30.4173647659547690   T   T   T
  3.8117039562017205 -0.8285946693289420 24.3290172400903018   T   T   T
  2.6063990590962605 -0.1384933757986515 26.3737661548724667   T   T   T
  2.5946762656965063 -1.5535222592102582 28.4117140945856335   T   T   T
  3.8140199966914197 -0.8508404397923414 30.4201218466540304   T   T   T
  5.0596125220278392  1.2887665015649985 24.3444484170166362   T   T   T
  3.8270651052361138  1.9923290406295904 26.4219480319033018   T   T   T
  3.8212544279786784  0.5687769289094563 28.4080017415414829   T   T   T
  5.0409640516144858  1.2723978686635835 30.4260885343911305   T   T   T
  2.6013334550278238  1.2608092737581773 24.4344280020303728   T   T   T
  1.3622036060894407  1.9931604229935618 26.4039956874880168   T   T   T
  1.3671741490588980  0.5681882733989468 28.3973773212607590   T   T   T
  2.5863687615214275  1.2715428806304183 30.4167826070783534   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_2x2/Ni E_tot= -221.26500749 eV
 D3-zero damping= -2.3267769 eV, D3-BJ damping= -3.3075729 eV
Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     4.9077161635400008    0.0000000000000000    0.0000000000000000
    -2.4538580817699986    4.2502068721891453    0.0000000000000000
     0.0000000000000018    0.0000000000000032   30.0121670387691815
   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.5307641245819466  0.1815383360119881  9.0169746245084816   F   F   F
 -1.2322782729352804  2.3444836289745989 10.8612336967246357   F   F   F
  2.2701965146094101  2.5907764880984683 11.6081185941916623   F   F   F
  3.4444681144570746  1.3958232918792568  9.5654178022134708   F   F   F
 -0.6201010982644807  3.7182176947390766 10.2987723773365900   F   F   F
  1.0920431130135873  3.3955149556354178  8.2518078419286844   F   F   F
 -0.1928577930664174  1.6985151526591546 11.9218080039603862   F   F   F
  2.5782530056722708 -0.0443305131806539 14.5050718430130097   F   F   F
  1.2076608772780650  1.9881722152178671 12.6701466762358947   F   F   F
 -1.3721707533769831  2.2353161456365340 16.3257721709636954   T   T   T
  2.0436430467843079  2.4466824372123419 16.9267050641496262   T   T   T
  3.5397008651786730  1.0828510920812924 15.1762937765250889   T   T   T
  1.7172143271210711  0.5943045897210512 13.2917821082657603   F   F   F
 -0.8713051051803534  3.6286630402924653 15.6574476934210640   T   T   T
  1.0455604563001411  3.0406735369437734 13.8903255655927005   F   F   F
 -0.4103226793459628  1.7894406838298376 17.5595766900408456   T   T   T
  0.1658742826946328  4.3523635740537667 19.9748996194167532   T   T   T
  1.0760649923422416  2.0275304744523663 18.1661638185387027   T   T   T
  3.7106644471944432  2.3205711782694278 21.8091134515997993   T   T   T
  3.5000315766871926  1.3582807707598596 20.5052468246468003   T   T   T
  1.5399635164402388  0.6392649123636818 18.8781050749972010   T   T   T
 -0.5475575509145074  3.7247835312188760 21.2967350409027532   T   T   T
  1.0982924140750858  3.2269598230942353 19.2688172683893448   T   T   T
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 -0.0995976481497730  1.5825386448280743 22.8010674447582993   T   T   T
  2.3563451238248829  2.8217249211219078 22.5690319828442334   T   T   T
  1.5514739443077794  2.2629250426630612 22.7268291742363466   T   T   T
 -0.1174244925353422  0.5961398858059220 22.8052773271139912   T   T   T
  1.3621914439617202  0.6727601662014105  8.0000000000000000   F   F   F
  1.1635345039674199  1.6337922032838519  8.0158744918591047   F   F   F
  1.9516775029748146  3.7962121098751287  8.0308754104330866   F   F   F

Oxidized reference: O-a-SiO2(0001)/fcc(111)_2x2/Ni E_tot= -208.5570791 eV
 D3-zero damping= -2.1913738 eV, D3-BJ damping= -3.1525339 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.9077161635400008    0.0000000000000000    0.0000000000000000
    -2.4538580817699986    4.2502068721891453    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.2344124266174816
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.5307641245819466  0.1815383360119881  9.0169746245084816   F   F   F
 -1.2322782729352804  2.3444836289745989 10.8612336967246357   F   F   F
  2.2701965146094101  2.5907764880984683 11.6081185941916623   F   F   F
  3.4444681144570746  1.3958232918792568  9.5654178022134708   F   F   F
 -0.6201010982644807  3.7182176947390766 10.2987723773365900   F   F   F
  1.0920431130135873  3.3955149556354178  8.2518078419286844   F   F   F
 -0.1928577930664174  1.6985151526591546 11.9218080039603862   F   F   F
  2.5782530056722708 -0.0443305131806539 14.5050718430130097   F   F   F
  1.2076608772780650  1.9881722152178671 12.6701466762358947   F   F   F
 -1.2099317536633758  2.1905911729762479 16.3662440698453722   T   T   T
  2.4104293082358392  2.4607866994190459 17.2973115858270994   T   T   T
  3.4995331221165231  1.0996436986364033 15.1871403100377957   T   T   T
  1.7172143271210711  0.5943045897210512 13.2917821082657603   F   F   F
 -0.8372794574118411  3.6108667925470490 15.6715762059841346   T   T   T
  1.0455604563001411  3.0406735369437734 13.8903255655927005   F   F   F
 -0.0437306717958276  1.6383793662092454 17.3457756965982099   T   T   T
 -0.1196778494570949  4.3148277035831120 20.1163879318491468   T   T   T
  1.1415644288076101  2.2475685313211149 18.2603913495245465   T   T   T
  4.1275832480368919  1.9290654236881168 21.8022268985359737   T   T   T
  3.3255862836508663  0.6456452758524587 21.2613654630524813   T   T   T
  1.3836196005226784  1.2321237629701614 19.5103982426157145   T   T   T
 -1.0648728833758805  3.1542076151107024 20.7690240757594466   T   T   T
  0.7412784073641938  3.6960774079322283 18.8825930301820399   T   T   T
  0.7339018138192415  1.7439138729223991 22.4137523478873106   T   T   T
  4.4030175018108952  2.1783854764950323 23.3949713084878184   T   T   T
  1.3621914439617202  0.6727601662014105  8.0000000000000000   F   F   F
  1.1635345039674199  1.6337922032838519  8.0158744918591047   F   F   F
  1.9516775029748146  3.7962121098751287  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_2x2/Ni E_tot= -86.86 eV
 D3-zero damping= -4.5388181 eV, D3-BJ damping= -5.6124263 eV
Ni
 1.0000000000000000
     4.9077161635400008    0.0000000000000000    0.0000000000000000
    -2.4538580817699986    4.2502068721891453    0.0000000000000000
     0.0000000000000023    0.0000000000000040   37.9724841506789446
  16
Cartesian
  6.2731439546597541 -0.8137750647428542 24.3589360139077939
  5.0387786807869563 -0.1017548068729220 26.3717295152474307
  5.0337512209505668 -1.5131407331504101 28.3822040145600134
  6.2572230703542910 -0.8033277889170880 30.3946952500141840
  3.8193767404973147 -0.8137295153513395 24.3592979547387216
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  2.5847637014375651 -0.1019926878381072 26.3712027059043841
  2.5797338396772318 -1.5130768521610694 28.3818866910215242
  3.8032387061770718 -0.8032874941768177 30.3943073566614288
  5.0463373648264156  1.3113766327719636 24.3591464467753624
  3.8117122625842117  2.0231723235350270 26.3711443486325194
  3.8065612137566815  0.6120087397121184 28.3818374096046071
  5.0301880756734647  1.3218052455879157 30.3941986633911583
  2.5924196959685921  1.3113886768859633 24.3590989169913996
  1.3579964725067355  2.0232789587503262 26.3715708792673169
  1.3527720869748519  0.6121974105099939 28.3823111592045869
  2.5764225099591740  1.3218036286128361 30.3947620480544032

Interface: O-a-SiO2(0001)/fcc(111)_2x2/Ir E_tot= -352.47659878 eV
 D3-zero damping= -10.8501471 eV, D3-BJ damping= -12.2576138 eV
Si  O Si  O Si  O  H Ir
 1.0000000000000000
     5.4301264291000013    0.0000000000000000    0.0000000000000000
    -2.7150632145499989    4.7026274333618812    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.6576454937617058
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.8001556530111156  0.2008624955935674  9.0169746245084816   F   F   F
 -1.3634502475067662  2.5940462105095188 10.8612336967246357   F   F   F
  2.5118514768260982  2.8665561355053528 11.6081185941916658   F   F   F
  3.8111204314257332  1.5444040965318837  9.5654178022134708   F   F   F
 -0.6861088233699051  4.1140097553617174 10.2987723773365900   F   F   F
  1.2082875154325106  3.7569563696406960  8.2518078419286880   F   F   F
 -0.2133868716711732  1.8793165116599810 11.9218080039603862   F   F   F
  2.8526995695099360 -0.0490493506992468 14.5050718430130097   F   F   F
  1.3362124109409623  2.1998066171107826 12.6701466762358947   F   F   F
 -1.2849933945737984  2.3795643447460981 16.1643699482698331   T   T   T
  2.7808201834933128  2.6347931497338211 17.0294725740838473   T   T   T
  3.7877928175869457  1.0915076502916266 15.1920400124046768   T   T   T
  1.9000061518234339  0.6575663612241029 13.2917821082657603   F   F   F
 -0.9077298446241943  3.8203471363291031 15.4620654781851812   T   T   T
  1.1568569325904086  3.3643432474533306 13.8903255655927040   F   F   F
  0.0544459993364539  1.9427298739405803 17.0027011921685691   T   T   T
  0.0035428279948547  4.6003563361698729 19.5403132610319652   T   T   T
  1.4112594620130039  2.2881041209300927 17.8615470433759533   T   T   T
  4.2199207340084435  2.1975045446288548 21.2559940075930562   T   T   T
  3.5721295273424247  0.9097990690475082 20.4943506202291204   T   T   T
  1.7364795597504934  0.9012882016753965 18.6859579700766325   T   T   T
 -0.9351117315683284  3.5013601883531789 20.3092127264705873   T   T   T
  1.0666498791472248  3.6696151084829887 18.6929490787935642   T   T   T
  0.1344483947096455  1.6884606697822593 22.0238964395340382   T   T   T
  3.1085499845039690  2.7817597236124318 22.3730397870296223   T   T   T
  1.5071922488718195  0.7443732761229832  8.0000000000000000   F   F   F
  1.2873889301303623  1.8077040169148444  8.0158744918591083   F   F   F
  2.1594271626212107  4.2003064198059352  8.0308754104330902   F   F   F
  6.7729490818160407 -0.8269835020097945 24.0465853386171631   T   T   T
  5.4032475053983804 -0.0161919635515917 26.2487293189219280   T   T   T
  5.4130593215595715 -1.6062754256589937 28.4730563182962548   T   T   T
  6.7815684050610017 -0.8160619512667640 30.6445837428562413   T   T   T
  4.0230216951409679 -0.7859136837178702 24.1004065382245258   T   T   T
  2.6713894617213807 -0.0182087290771658 26.1986482589818017   T   T   T
  2.6998128546412183 -1.6088436871490568 28.4568536016918898   T   T   T
  4.0567000058492928 -0.8205711801592640 30.6574231803838444   T   T   T
  5.4580779763006460  1.5272786512234371 24.0315577918038983   T   T   T
  4.0530820710298485  2.3219447305832284 26.2662903206410583   T   T   T
  4.0569300554096115  0.7434433234009848 28.4459247581730637   T   T   T
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  5.4194767257078036  1.5249588070850382 30.6306161958157048   T   T   T
  2.7204493544131099  1.5367846798708069 24.0507230777171657   T   T   T
  1.3295104854225397  2.3258408825791892 26.2562637898649278   T   T   T
  1.3454834491841612  0.7420235312343769 28.4258347044914075   T   T   T
  2.6990997719349030  1.5143658295492330 30.6407134282943616   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_2x2/Ir E_tot= -217.47174269 eV
 D3-zero damping= -1.8836732 eV, D3-BJ damping= -2.7156419 eV
Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     5.4301264291000013    0.0000000000000000    0.0000000000000000
    -2.7150632145499989    4.7026274333618812    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.3957697805030485
   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.8001556530111156  0.2008624955935674  9.0169746245084816   F   F   F
 -1.3634502475067662  2.5940462105095188 10.8612336967246357   F   F   F
  2.5118514768260982  2.8665561355053528 11.6081185941916623   F   F   F
  3.8111204314257332  1.5444040965318837  9.5654178022134708   F   F   F
 -0.6861088233699051  4.1140097553617174 10.2987723773365900   F   F   F
  1.2082875154325106  3.7569563696406960  8.2518078419286844   F   F   F
 -0.2133868716711732  1.8793165116599810 11.9218080039603862   F   F   F
  2.8526995695099360 -0.0490493506992468 14.5050718430130097   F   F   F
  1.3362124109409623  2.1998066171107826 12.6701466762358947   F   F   F
 -1.2724656536034382  2.3760894852466028 16.1649110115019248   T   T   T
  2.7993932231417564  2.6388892140310807 17.0395135530147641   T   T   T
  3.7873510887540096  1.0930327762266336 15.1915490145138463   T   T   T
  1.9000061518234339  0.6575663612241029 13.2917821082657603   F   F   F
 -0.9017345326951638  3.8207506166919982 15.4674517486792240   T   T   T
  1.1568569325904086  3.3643432474533306 13.8903255655927005   F   F   F
  0.0771401821040206  1.9325395722631975 16.9874140546300829   T   T   T
  0.0669394941263044  4.6495995202547311 19.5566252820664452   T   T   T
  1.4235822550051471  2.2863843684054483 17.8606330853478603   T   T   T
  4.1672671756849864  2.2929122792141503 21.2919900456116586   T   T   T
  3.7233619289110109  0.9825004017216752 20.4035463130323222   T   T   T
  1.7622523929579381  0.9153673840417069 18.7033105019462162   T   T   T
 -0.8503561706057317  3.6467886628893900 20.4638139355194220   T   T   T
  1.0577376518017823  3.6558905117794813 18.6974946273895810   T   T   T
  0.1281853672745585  1.8594322687080234 22.0871747678000396   T   T   T
  2.9643538506645788  2.7316539191846028 22.3049805508272563   T   T   T
  2.0423745747497577  2.4148133647688161 22.1839302295990741   T   T   T
  0.1386319531172946  0.9323617084525143 22.3918719748881259   T   T   T
  1.5071922488718195  0.7443732761229832  8.0000000000000000   F   F   F
  1.2873889301303623  1.8077040169148444  8.0158744918591047   F   F   F
  2.1594271626212107  4.2003064198059352  8.0308754104330866   F   F   F

Oxidized reference: O-a-SiO2(0001)/fcc(111)_2x2/Ir E_tot= -204.97641103 eV
 D3-zero damping= -1.8117326 eV, D3-BJ damping= -2.6475643 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     5.4301264291000013    0.0000000000000000    0.0000000000000000
    -2.7150632145499989    4.7026274333618812    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.2989605531014377
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.8001556530111156  0.2008624955935674  9.0169746245084816   F   F   F
 -1.3634502475067662  2.5940462105095188 10.8612336967246357   F   F   F
  2.5118514768260982  2.8665561355053528 11.6081185941916623   F   F   F
  3.8111204314257332  1.5444040965318837  9.5654178022134708   F   F   F
 -0.6861088233699051  4.1140097553617174 10.2987723773365900   F   F   F
  1.2082875154325106  3.7569563696406960  8.2518078419286844   F   F   F
```

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 -0.2133868716711732  1.8793165116599810 11.9218080039603862   F   F   F
  2.8526995695099360 -0.0490493506992468 14.5050718430130097   F   F   F
  1.3362124109409623  2.1998066171107826 12.6701466762358947   F   F   F
 -1.2731971316596671  2.3745029005032019 16.1641293385697971   T   T   T
  2.7970749522232072  2.6322503678870155 17.0401618263325432   T   T   T
  3.7896040187624069  1.0908510158069080 15.1931464795157165   T   T   T
  1.9000061518234339  0.6575663612241029 13.2917821082657603   F   F   F
 -0.9003516536479556  3.8203776707048500 15.4718034108297946   T   T   T
  1.1568569325904086  3.3643432474533306 13.8903255655927005   F   F   F
  0.0712722370454097  1.9308475474920110 16.9960632375166831   T   T   T
  0.0138979539706811  4.6108181880492030 19.5544681801627860   T   T   T
  1.4224341059844188  2.2899590511255208 17.8613048906606160   T   T   T
  4.6297699122083751  2.0582184788934024 21.0457347701110287   T   T   T
  3.6470402827044244  0.9196451425854750 20.4601007871680665   T   T   T
  1.7420578518199288  0.9153489412655197 18.7109533651346283   T   T   T
 -0.9566859273406583  3.5174525990779069 20.3245114328682668   T   T   T
  1.0503724794606566  3.6655140514144167 18.6883739906267756   T   T   T
  0.7349363391567787  1.6348817303726495 21.4681751711057451   T   T   T
  5.0668656018809379  1.9998639469667514 22.6245831115162197   T   T   T
  1.5071922488718195  0.7443732761229832  8.0000000000000000   F   F   F
  1.2873889301303623  1.8077040169148444  8.0158744918591047   F   F   F
  2.1594271626212107  4.2003064198059352  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_2x2/Ir E_tot= -142.55139983 eV
 D3-zero damping= -8.1348177 eV, D3-BJ damping= -8.6989163 eV
Ir
 1.0000000000000000
     5.4301264291000013    0.0000000000000000    0.0000000000000000
    -2.7150632145499989    4.7026274333618812    0.0000000000000000
     0.0000000000000014    0.0000000000000024   22.6258653885799426
  16
Cartesian
  6.7712451451765174 -0.8157252575316434  8.0269848009643461
  5.4143948710424850 -0.0326119016926160 10.2233223814451399
  5.4143809338233924 -1.6012817385359230 12.4102934973253518
  6.7711571719837540 -0.8182746878181311 14.6065939151788484
  4.0563223395233603 -0.8160069740441912  8.0274799111249546
  2.6991839857265294 -0.0327940658212822 10.2235354784701205
  2.6992909488314671 -1.6014998129292135 12.4102708893628542
  4.0561258428484672 -0.8182045239874425 14.6069700659546164
  5.4135002427671539  1.5354513209641238  8.0267430006490876
  4.0568771525197649  2.3183755727694266 10.2231004438943849
  4.0570212485476143  0.7502385701636866 12.4103125575873552
  5.4138962389202767  1.5330097958233169 14.6064763994947722
  2.6985148897476949  1.5354414425844916  8.0269560952847954
  1.3415529321606587  2.3182536921510484 10.2232371510180897
  1.3417386384045433  0.7501336057448693 12.4103358295656854
  2.6986552920537865  1.5330853719259310 14.6066737113174536

Interface: O-a-SiO2(0001)/fcc(111)_2x2/Rh E_tot= -327.95003828 eV
 D3-zero damping= -9.3534786 eV, D3-BJ damping= -11.399847 eV
Si  O Si  O Si  O  H Rh
 1.0000000000000000
     5.3553253905600009    0.0000000000000000    0.0000000000000000
    -2.6776626952799987    4.6378478337567817    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.6065551851437192
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.7615829689946958  0.1980955759885988  9.0169746245084816   F   F   F
 -1.3446684574614043  2.5583127238033860 10.8612336967246357   F   F   F
  2.4772502384243680  2.8270687720399410 11.6081185941916658   F   F   F
  3.7586215126631894  1.5231296323266068  9.5654178022134708   F   F   F
```

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 -0.6766575420397882  4.0573384777620616 10.2987723773365900   F   F   F
  1.1916431219382970  3.7052035712725790  8.2518078419286880   F   F   F
 -0.2104474263709187  1.8534285643620694 11.9218080039603862   F   F   F
  2.8134030829127861 -0.0483736864361912 14.5050718430130097   F   F   F
  1.3178058273460040  2.1695038568167972 12.6701466762358947   F   F   F
 -1.2796752160829443  2.3529069938168941 16.1976230424267911   T   T   T
  2.7141738622090825  2.6059439129479451 17.0587636651735863   T   T   T
  3.7469965860738275  1.0906444269038988 15.1917522488681200   T   T   T
  1.8738332007431147  0.6485082578132981 13.2917821082657603   F   F   F
 -0.8995240624330314  3.7862450773775089 15.4908534319620053   T   T   T
  1.1409210052911423  3.3179987705428258 13.8903255655927040   F   F   F
  0.0293896425779737  1.9090288172052796 17.0704299098050605   T   T   T
 -0.0178575464857584  4.5299442418193143 19.6499955654342244   T   T   T
  1.3765056368543449  2.2627851404350450 17.9328108773079791   T   T   T
  4.1914231267399957  2.1444572285867807 21.3757843431696415   T   T   T
  3.5008116826819959  0.8537003324302128 20.6606952057673254   T   T   T
  1.7068774271791329  0.9027664608571918 18.7847563285770498   T   T   T
 -0.9787892056793825  3.4313501145334846 20.3874290449884832   T   T   T
  1.0474777666588417  3.6309969807593778 18.7805288329491873   T   T   T
  0.2399280129577167  1.6818644070753095 22.0604710067793093   T   T   T
  3.1360671006206564  2.7149899838411726 22.5645699575524681   T   T   T
  1.4864303850428520  0.7341193907222614  8.0000000000000000   F   F   F
  1.2696548993971934  1.7828025455396055  8.0158744918591047   F   F   F
  2.1296806370983559  4.1424463890147569  8.0308754104330866   F   F   F
  6.9745052484123491 -0.9751077628700446 24.0946393590410075   T   T   T
  5.6271073403811469 -0.2072938596637687 26.2488596107327226   T   T   T
  5.6358098307124100 -1.7779763418623256 28.4354454151743674   T   T   T
  6.9809207992687261 -1.0015864092779287 30.5826108408460016   T   T   T
  4.2783297650499232 -0.9832670140346330 24.0752800375360501   T   T   T
  2.9587294906570452 -0.2252306551588899 26.1935395485953535   T   T   T
  2.9596199464915043 -1.7723440914086017 28.4185042012426443   T   T   T
  4.2980529972072885 -1.0023750643093106 30.5895319265098529   T   T   T
  5.6352029328530859  1.3291939173097354 24.0317821139389309   T   T   T
  4.2914349563884064  2.0985896737886658 26.2794013679667238   T   T   T
  4.2923494425022950  0.5367527393921477 28.4127938515933138   T   T   T
  5.6396704954853041  1.3142601920138597 30.5782831302143805   T   T   T
  2.9501874285759677  1.3028159975019831 24.0943268370159416   T   T   T
  1.6070156958119008  2.0975834805073976 26.2644731909170197   T   T   T
  1.6266099934313780  0.5357073855850033 28.3958302683430261   T   T   T
  2.9611873738829515  1.3074324074889914 30.5809082675502353   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_2x2/Rh E_tot= -218.51626679 eV
 D3-zero damping= -1.928709 eV, D3-BJ damping= -2.772251 eV
Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     5.3553253905600009    0.0000000000000000    0.0000000000000000
    -2.6776626952799987    4.6378478337567817    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.5109872735401986
   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.7615829689946958  0.1980955759885988  9.0169746245084816   F   F   F
 -1.3446684574614043  2.5583127238033860 10.8612336967246357   F   F   F
  2.4772502384243680  2.8270687720399410 11.6081185941916623   F   F   F
  3.7586215126631894  1.5231296323266068  9.5654178022134708   F   F   F
 -0.6766575420397882  4.0573384777620616 10.2987723773365900   F   F   F
  1.1916431219382970  3.7052035712725790  8.2518078419286844   F   F   F
 -0.2104474263709187  1.8534285643620694 11.9218080039603862   F   F   F
  2.8134030829127861 -0.0483736864361912 14.5050718430130097   F   F   F
  1.3178058273460040  2.1695038568167972 12.6701466762358947   F   F   F
 -1.2571890843733740  2.3459239834982615 16.1999532727110207   T   T   T
  2.7566857344360161  2.5986934850433601 17.0937172252079499   T   T   T
  3.7437995926447978  1.0893738533791433 15.1976319029089293   T   T   T
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  1.8738332007431147  0.6485082578132981 13.2917821082657603   F   F   F
 -0.8958124465258841  3.7833150892437155 15.4929818606937619   T   T   T
  1.1409210052911423  3.3179987705428258 13.8903255655927005   F   F   F
  0.0725659477969795  1.8910817228684587 17.0386515149336830   T   T   T
  0.0702070482533897  4.5830315033454205 19.6634179908676785   T   T   T
  1.3984404777257800  2.2436393090506779 17.9321677633325010   T   T   T
  4.1193880416352675  2.2542647509079647 21.4304226068184214   T   T   T
  3.6961412228935782  0.9710136137424035 20.5038604435128207   T   T   T
  1.7253378310639216  0.8917982024939729 18.7991464953486336   T   T   T
 -0.8295939949524220  3.6082584382213998 20.6089606380400845   T   T   T
  1.0404487435080236  3.5983849711881599 18.7838073575507174   T   T   T
  0.1496892272860450  1.8092838181271258 22.2301801433280950   T   T   T
  2.9142657889247636  2.6799181776425134 22.4424657642138428   T   T   T
  1.9893585468274491  2.3638223353316672 22.3248702029539920   T   T   T
  0.1617147511031318  0.8759195802776235 22.5167965602665703   T   T   T
  1.4864303850428520  0.7341193907222614  8.0000000000000000   F   F   F
  1.2696548993971934  1.7828025455396055  8.0158744918591047   F   F   F
  2.1296806370983559  4.1424463890147569  8.0308754104330866   F   F   F

Oxidized reference: O-a-SiO2(0001)/fcc(111)_2x2/Rh E_tot= -206.00371904 eV
 D3-zero damping= -1.8534919 eV, D3-BJ damping= -2.6991929 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     5.3553253905600009    0.0000000000000000    0.0000000000000000
    -2.6776626952799987    4.6378478337567817    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.2989605531014377
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.7615829689946958  0.1980955759885988  9.0169746245084816   F   F   F
 -1.3446684574614043  2.5583127238033860 10.8612336967246357   F   F   F
  2.4772502384243680  2.8270687720399410 11.6081185941916623   F   F   F
  3.7586215126631894  1.5231296323266068  9.5654178022134708   F   F   F
 -0.6766575420397882  4.0573384777620616 10.2987723773365900   F   F   F
  1.1916431219382970  3.7052035712725790  8.2518078419286844   F   F   F
 -0.2104474263709187  1.8534285643620694 11.9218080039603862   F   F   F
  2.8134030829127861 -0.0483736864361912 14.5050718430130097   F   F   F
  1.3178058273460040  2.1695038568167972 12.6701466762358947   F   F   F
 -1.2542242282352405  2.3434546900219013 16.1986370137315276   T   T   T
  2.7592847008395021  2.5917051741770196 17.0949662961454720   T   T   T
  3.7473077907803791  1.0899205201046873 15.1949083497214836   T   T   T
  1.8738332007431147  0.6485082578132981 13.2917821082657603   F   F   F
 -0.8909427601420217  3.7851442063121437 15.5018658045134181   T   T   T
  1.1409210052911423  3.3179987705428258 13.8903255655927005   F   F   F
  0.0709111708509481  1.8887754222421460 17.0470572786512378   T   T   T
  0.0075003808551710  4.5456886313641869 19.6616999169610125   T   T   T
  1.3981256485765661  2.2626278006230023 17.9323623894021829   T   T   T
  4.5659866709647838  2.0221652156473033 21.1936062299713335   T   T   T
  3.6005447979860663  0.8705290015440882 20.6120981503359388   T   T   T
  1.7050123911473956  0.9232725548940623 18.8300228520847028   T   T   T
 -0.9598074139370617  3.4496819549948143 20.4216446989471194   T   T   T
  1.0308773996085894  3.6365415783536381 18.7535059629628513   T   T   T
  0.7423237614066293  1.6234704266942965 21.6500116914125869   T   T   T
  4.9777955680838684  2.0069425909893606 22.7794927801412825   T   T   T
  1.4864303850428520  0.7341193907222614  8.0000000000000000   F   F   F
  1.2696548993971934  1.7828025455396055  8.0158744918591047   F   F   F
  2.1296806370983559  4.1424463890147569  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_2x2/Rh E_tot= -116.53749289 eV
 D3-zero damping= -6.6124321 eV, D3-BJ damping= -7.8068863 eV
Rh
 1.0000000000000000
     5.3553253905600009    0.0000000000000000    0.0000000000000000
```

```
    -2.6776626952799987    4.6378478337567817    0.0000000000000000
     0.0000000000000014    0.0000000000000024   22.5577498125709184
  16
Cartesian
  6.9719368193375431 -0.9936927321549207  8.0501285459611331
  5.6316423080387334 -0.2243309294167380 10.2235899601703721
  5.6331280527402861 -1.7730544763853324 12.3723008453781311
  6.9757704301849790 -1.0026471565187984 14.5448869462869137
  4.2939042339324596 -0.9936178554523988  8.0501842874561138
  2.9538316448199842 -0.2239191591605812 10.2237073440920092
  2.9557366847336586 -1.7728477350503007 12.3727807934437024
  4.2981664303219240 -1.0025953596586712 14.5451758216929665
  5.6325569620864586  1.3247979772037972  8.0511186000488095
  4.2924476838365226  2.0949215208411052 10.2236425499857795
  4.2943248795820352  0.5456080416916375 12.3728660723310693
  5.6369571988572780  1.3163146566147557 14.5456627766010911
  2.9550133231200904  1.3250745260050767  8.0502054854508973
  1.6152511235107787  2.0950914855350105 10.2234980502304378
  1.6168105482917354  0.5457328129644571 12.3729100782526089
  2.9592555083921441  1.3163191108611134 14.5450379884744034

Interface: O-a-SiO2(0001)/fcc(111)_2x2/Os E_tot= -386.65828744 eV
 D3-zero damping= -9.2127815 eV, D3-BJ damping= -11.1320489 eV
Si  O Si  O Si  O  H Os
 1.0000000000000000
     5.4168285661600013    0.0000000000000000    0.0000000000000000
    -2.7084142830799989    4.6911111462397974    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.6202765539586608
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.7932983382560006  0.2003706024542335  9.0169746245084799   F   F   F
 -1.3601112875850063  2.5876936381674600 10.8612336967246339   F   F   F
  2.5057001915658752  2.8595362122867169 11.6081185941916640   F   F   F
  3.8017873601231309  1.5406219978518976  9.5654178022134690   F   F   F
 -0.6844286081457800  4.1039349369251799 10.2987723773365882   F   F   F
  1.2053285342776283  3.7477559409716115  8.2518078419286862   F   F   F
 -0.2128643075265389  1.8747142443427767 11.9218080039603844   F   F   F
  2.8457135797029491 -0.0489292335065053 14.5050718430130079   F   F   F
  1.3329401538892303  2.1944195000204547 12.6701466762358930   F   F   F
 -1.2874393648909621  2.3759443661189663 16.1681196011216457   T   T   T
  2.7615929558822248  2.6321640527114365 17.0247263239698547   T   T   T
  3.7815771791915078  1.0928669948340495 15.1882572729382481   T   T   T
  1.8953532175461205  0.6559560437739137 13.2917821082657586   F   F   F
 -0.9050430601598419  3.8162527960021304 15.4693334558206370   T   T   T
  1.1540239000392076  3.3561042909627421 13.8903255655927023   F   F   F
  0.0427300905335508  1.9370762771775580 17.0179999705642544   T   T   T
  0.0139078115255198  4.6082960154137842 19.5540692096195272   T   T   T
  1.4006902261723271  2.2897313463784688 17.8701182057130694   T   T   T
  4.2248023933288694  2.2087717780277991 21.2731796164164706   T   T   T
  3.5943528320325226  0.9281780580544006 20.4895238665079837   T   T   T
  1.7306038181181918  0.9140816456703754 18.7066896924023780   T   T   T
 -0.9197234443504985  3.5228710643410337 20.3438105375327716   T   T   T
  1.0626487990874245  3.6732825984073059 18.6970672547364103   T   T   T
  0.1559425249278746  1.6958587528873879 22.0375308899137643   T   T   T
  3.1231170183453738  2.7590343906138575 22.4128487622228434   T   T   T
  1.5035012784659885  0.7425503767980178  7.9999999999999982   F   F   F
  1.2842362371375060  1.8032771217832320  8.0158744918591065   F   F   F
  2.1541389309727612  4.1900202690494339  8.0308754104330884   F   F   F
  6.8586890193803871 -0.8992722676067442 24.1116130944996634   T   T   T
  5.5355360523643755 -0.0896165895359964 26.2121021074479046   T   T   T
  5.5432997186298527 -1.6786866072328266 28.5023944019407338   T   T   T
  6.8775924733075779 -0.9018780464043282 30.6154558422587613   T   T   T
```

```
  4.1646907520980880 -0.8702527529210822 24.1465453042367244   T   T   T
  2.8318841491004738 -0.1291716374646961 26.2078156626109653   T   T   T
  2.8271565638742153 -1.6717704186718096 28.4862873657535545   T   T   T
  4.1795843862986084 -0.8970492018046318 30.6201925396729457   T   T   T
  5.5569678740200326  1.4594439806463391 24.0301340119196389   T   T   T
  4.1991977756261019  2.2045916466020179 26.2155552226820525   T   T   T
  4.1784431236376189  0.6701937827337302 28.4862346844497445   T   T   T
  5.5319577679175547  1.4537784254761741 30.6098769324761228   T   T   T
  2.8309418490056819  1.4724212220728372 24.1047105551563448   T   T   T
  1.4471239943469920  2.2091804082255120 26.2194040757386198   T   T   T
  1.4752973650282830  0.6702694366678554 28.4959484240516900   T   T   T
  2.8258410358529424  1.4625535764336353 30.6143297484036587   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_2x2/Os E_tot= -217.67046571 eV
 D3-zero damping= -1.8909073 eV, D3-BJ damping= -2.7245002 eV
Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     5.4168285661600013    0.0000000000000000    0.0000000000000000
    -2.7084142830799989    4.6911111462397974    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.4213310303273055
   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.7932983382560006  0.2003706024542335  9.0169746245084816   F   F   F
 -1.3601112875850063  2.5876936381674600 10.8612336967246357   F   F   F
  2.5057001915658752  2.8595362122867169 11.6081185941916623   F   F   F
  3.8017873601231309  1.5406219978518976  9.5654178022134708   F   F   F
 -0.6844286081457800  4.1039349369251799 10.2987723773365900   F   F   F
  1.2053285342776283  3.7477559409716115  8.2518078419286844   F   F   F
 -0.2128643075265389  1.8747142443427767 11.9218080039603862   F   F   F
  2.8457135797029491 -0.0489292335065053 14.5050718430130097   F   F   F
  1.3329401538892303  2.1944195000204547 12.6701466762358947   F   F   F
 -1.2692164562184949  2.3696282759038287 16.1734016466775827   T   T   T
  2.7925132428902195  2.6295285169054505 17.0520121467145742   T   T   T
  3.7804576383739095  1.0897414761954149 15.1961310253949886   T   T   T
  1.8953532175461205  0.6559560437739137 13.2917821082657603   F   F   F
 -0.8996540793005190  3.8126811141300632 15.4731000284663232   T   T   T
  1.1540239000392076  3.3561042909627421 13.8903255655927005   F   F   F
  0.0776448154744742  1.9258545846429660 16.9984102095338976   T   T   T
  0.0708190620836902  4.6414524677983584 19.5797289748397496   T   T   T
  1.4190445456594531  2.2801035506559755 17.8766527462139209   T   T   T
  4.1645230134926265  2.2874781192418205 21.3206822454283014   T   T   T
  3.7254946113026093  0.9848618690426229 20.4206082966635059   T   T   T
  1.7550902651147482  0.9142019113168935 18.7275643719627105   T   T   T
 -0.8385765912963552  3.6436012700984355 20.4985492012707979   T   T   T
  1.0550730473846766  3.6484861605067391 18.7141238434877373   T   T   T
  0.1347052375188693  1.8494398293414027 22.1208946176810670   T   T   T
  2.9577121961991506  2.7239019891469041 22.3288735478278149   T   T   T
  2.0353029554811739  2.4070976457465338 22.2090451823410397   T   T   T
  0.1452211784468072  0.9206931421933208 22.4211123941856094   T   T   T
  1.5035012784659885  0.7425503767980178  8.0000000000000000   F   F   F
  1.2842362371375060  1.8032771217832320  8.0158744918591047   F   F   F
  2.1541389309727612  4.1900202690494339  8.0308754104330866   F   F   F

Oxidized reference: O-a-SiO2(0001)/fcc(111)_2x2/Os E_tot= -205.170253 eV
 D3-zero damping= -1.8186335 eV, D3-BJ damping= -2.6559189 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     5.4168285661600013    0.0000000000000000    0.0000000000000000
    -2.7084142830799989    4.6911111462397974    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.2989605531014377
   2   5   3   6   3   7   2
Selective dynamics
```

```
Cartesian
  2.7932983382560006  0.2003706024542335  9.0169746245084816   F   F   F
 -1.3601112875850063  2.5876936381674600 10.8612336967246357   F   F   F
  2.5057001915658752  2.8595362122867169 11.6081185941916623   F   F   F
  3.8017873601231309  1.5406219978518976  9.5654178022134708   F   F   F
 -0.6844286081457800  4.1039349369251799 10.2987723773365900   F   F   F
  1.2053285342776283  3.7477559409716115  8.2518078419286844   F   F   F
 -0.2128643075265389  1.8747142443427767 11.9218080039603862   F   F   F
  2.8457135797029491 -0.0489292335065053 14.5050718430130097   F   F   F
  1.3329401538892303  2.1944195000204547 12.6701466762358947   F   F   F
 -1.2661083971483080  2.3675679614804168 16.1697049864376545   T   T   T
  2.7962206941767556  2.6213573524908278 17.0529974063937146   T   T   T
  3.7828165502678734  1.0909429814045524 15.1921521936678836   T   T   T
  1.8953532175461205  0.6559560437739137 13.2917821082657603   F   F   F
 -0.8978886795898835  3.8145890383924224 15.4785188555974784   T   T   T
  1.1540239000392076  3.3561042909627421 13.8903255655927005   F   F   F
  0.0767051204052497  1.9213380779396318 17.0008600680649202   T   T   T
  0.0144617707260330  4.5999843565720866 19.5723462582369088   T   T   T
  1.4207961823996431  2.2852127253393810 17.8729485657559835   T   T   T
  4.6189277476554862  2.0520994737996503 21.0745402058775362   T   T   T
  3.6400536289313363  0.9127728529457585 20.4851746625608158   T   T   T
  1.7346325398331934  0.9178799002198793 18.7343295697591010   T   T   T
 -0.9524807641200177  3.5047773378771421 20.3419876661592021   T   T   T
  1.0470704240786792  3.6615234225612898 18.6960967484831819   T   T   T
  0.7336679992920433  1.6291599957885641 21.5100032725839583   T   T   T
  5.0452452325034152  2.0007030340995970 22.6565895696049999   T   T   T
  1.5035012784659885  0.7425503767980178  8.0000000000000000   F   F   F
  1.2842362371375060  1.8032771217832320  8.0158744918591047   F   F   F
  2.1541389309727612  4.1900202690494339  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_2x2/Os E_tot= -175.54015681 eV
 D3-zero damping= -6.5637345 eV, D3-BJ damping= -7.5809275 eV
Os
 1.0000000000000000
     5.4168285661600013    0.0000000000000000    0.0000000000000000
    -2.7084142830799989    4.6911111462397974    0.0000000000000000
     0.0000000000000014    0.0000000000000024   22.5900585277533068
  16
Cartesian
  6.8883290519983973 -0.8936002816578233  8.0631501878468228
  5.5330428038214672 -0.1111990169978003 10.2010541766017955
  5.5333183598417426 -1.6752920646191458 12.4483673560490846
  6.8875539783672801 -0.8936805876825404 14.5866679964647989
  4.1792451418485053 -0.8939694269524900  8.0628545496053370
  2.8242165324370436 -0.1112901693365837 10.2003690755799337
  2.8247964982753690 -1.6754727978349417 12.4484859983565599
  4.1786644209693051 -0.8938218936084958 14.5867246052227593
  5.5338863426785245  1.4515058506486429  8.0629635997554523
  4.1789207816560499  2.2339334672858251 10.2013995218592051
  4.1789781971393927  0.6701247660749936 12.4484774005831458
  5.5328919527219709  1.4515590894359240 14.5863340173604357
  2.8253818949396758  1.4510428929043406  8.0631652224239563
  1.4700101564841845  2.2336467509562623 10.2009157220734554
  1.4705372679439088  0.6701613497748945 12.4489367943271372
  2.8244304868607291  1.4510868904074519 14.5865896147746454

Interface: O-a-SiO2(0001)/fcc(111)_2x2/Ru E_tot= -357.53528052 eV
 D3-zero damping= -9.0206877 eV, D3-BJ damping= -11.0855355 eV
Si  O Si  O Si  O  H Ru
 1.0000000000000000
     5.3323894838800010    0.0000000000000000    0.0000000000000000
    -2.6661947419399987    4.6179847559130724    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.6032777666756743
```

```
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.7497556000401238  0.1972471678502988  9.0169746245084834   F   F   F
 -1.3389094814876494  2.5473559251754549 10.8612336967246375   F   F   F
  2.4666406160115706  2.8149609390317449 11.6081185941916676   F   F   F
  3.7425240048606119  1.5166063388643334  9.5654178022134726   F   F   F
 -0.6737595380705244  4.0399616182981788 10.2987723773365918   F   F   F
  1.1865395262746576  3.6893348430173525  8.2518078419286898   F   F   F
 -0.2095461174531081  1.8454906592881426 11.9218080039603880   F   F   F
  2.8013537776218964 -0.0481665105361378 14.5050718430130114   F   F   F
  1.3121618992419066  2.1602122574511333 12.6701466762358965   F   F   F
 -1.2585375924364595  2.3402406662989774 16.2098058661739124   T   T   T
  2.7320945758593576  2.5906346327735084 17.0997586065377121   T   T   T
  3.7329850677593281  1.0898080446878236 15.1957513256340704   T   T   T
  1.8658079062387156  0.6457308122245325 13.2917821082657621   F   F   F
 -0.8966212335068816  3.7747062320632048 15.4988173122438386   T   T   T
  1.1360346434366904  3.3037883716192287 13.8903255655927058   F   F   F
  0.0600334750584503  1.8936363003538170 17.0648286859252103   T   T   T
 -0.0113407212966476  4.5002658224648364 19.6892819470842468   T   T   T
  1.3866159919083236  2.2431179674884123 17.9573911514710503   T   T   T
  4.1376171481637218  2.1441975102858448 21.4368192918850688   T   T   T
  3.5041006246425312  0.8409546515573650 20.6940960159132459   T   T   T
  1.7039616147082899  0.8849741163038879 18.8145724662316915   T   T   T
 -0.9768256110293622  3.4215234146051072 20.4451684143327022   T   T   T
  1.0453766090859593  3.5982227389284045 18.8164319011184311   T   T   T
  0.1886843936434630  1.6982472956002610 22.1792409478276085   T   T   T
  3.0587386781066597  2.6851526925162075 22.6028437782368954   T   T   T
  1.4800642679330018  0.7309752878695637  8.0000000000000018   F   F   F
  1.2642171931581458  1.7751671191497465  8.0158744918591101   F   F   F
  2.1205595935037325  4.1247050274958426  8.0308754104330919   F   F   F
  6.8606103774281406 -0.9888192990146595 24.2174307794996970   T   T   T
  5.5546192742037865 -0.2128520237274574 26.2537660441273815   T   T   T
  5.5548161874726674 -1.7817423899309057 28.5451365814754396   T   T   T
  6.8676941214272285 -1.0107957184981424 30.5999093785489897   T   T   T
  4.2280225492809942 -1.0017012965204628 24.2093664931283250   T   T   T
  2.9052327714749624 -0.2623576117857752 26.2784778271399766   T   T   T
  2.8832312835438114 -1.7816610659829140 28.5175791434760519   T   T   T
  4.2254709288844516 -1.0144977713526875 30.6054918978269015   T   T   T
  5.5559005347528636  1.3174139059706540 24.1384467549151189   T   T   T
  4.2393066911943276  2.0389710926907036 26.2694520698553760   T   T   T
  4.2189104805738715  0.5449914498761551 28.5174535119428967   T   T   T
  5.5490690483991294  1.3060022600979460 30.6050740438898856   T   T   T
  2.8757312817443141  1.3062212346942157 24.2098786083229882   T   T   T
  1.5240766815677642  2.0413777629913450 26.2606115452735907   T   T   T
  1.5440931360228503  0.5438929642411774 28.5274371031634111   T   T   T
  2.8766818320051835  1.3193662092230991 30.6029452070428931   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_2x2/Ru E_tot= -218.80965088 eV
 D3-zero damping= -1.9423992 eV, D3-BJ damping= -2.7894714 eV
Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     5.3323894838800010    0.0000000000000000    0.0000000000000000
    -2.6661947419399987    4.6179847559130724    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.5342538045973697
   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.7497556000401238  0.1972471678502988  9.0169746245084816   F   F   F
 -1.3389094814876494  2.5473559251754549 10.8612336967246357   F   F   F
  2.4666406160115706  2.8149609390317449 11.6081185941916623   F   F   F
  3.7425240048606119  1.5166063388643334  9.5654178022134708   F   F   F
 -0.6737595380705244  4.0399616182981788 10.2987723773365900   F   F   F
```

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  1.1865395262746576  3.6893348430173525  8.2518078419286844   F   F   F
 -0.2095461174531081  1.8454906592881426 11.9218080039603862   F   F   F
  2.8013537776218964 -0.0481665105361378 14.5050718430130097   F   F   F
  1.3121618992419066  2.1602122574511333 12.6701466762358947   F   F   F
 -1.2528485160135585  2.3368353763180894 16.2126253203062021   T   T   T
  2.7410180030444988  2.5850030464616247 17.1094296912559685   T   T   T
  3.7321413961420533  1.0888390391930798 15.1992503826876053   T   T   T
  1.8658079062387156  0.6457308122245325 13.2917821082657603   F   F   F
 -0.8911607037227637  3.7728187346561359 15.5047208486676169   T   T   T
  1.1360346434366904  3.3037883716192287 13.8903255655927005   F   F   F
  0.0677638225791245  1.8806252641747132 17.0620848300704218   T   T   T
  0.0780398235512543  4.5757629983872317 19.6999869416696924   T   T   T
  1.3890924276414822  2.2372367166332743 17.9579373154419919   T   T   T
  4.1101484451171331  2.2532728172185750 21.4772775975422725   T   T   T
  3.7007786302124792  0.9854220036484669 20.5265383541714286   T   T   T
  1.7108899002289726  0.8945077350612545 18.8393215843003503   T   T   T
 -0.8035053154431462  3.6104708862363086 20.6698487886434705   T   T   T
  1.0356550175559385  3.5923980894930083 18.8080309729526434   T   T   T
  0.1512311113934112  1.7952430808726947 22.2909868937843001   T   T   T
  2.8952153722947993  2.6799967822513224 22.4760128345472019   T   T   T
  1.9723713513713701  2.3536973167353654 22.3658876928191042   T   T   T
  0.1608192447866433  0.8569442959588969 22.5620530579127951   T   T   T
  1.4800642679330018  0.7309752878695637  8.0000000000000000   F   F   F
  1.2642171931581458  1.7751671191497465  8.0158744918591047   F   F   F
  2.1205595935037325  4.1247050274958426  8.0308754104330866   F   F   F

Oxidized reference: O-a-SiO2(0001)/fcc(111)_2x2/Ru E_tot= -206.294983 eV
 D3-zero damping= -1.8668986 eV, D3-BJ damping= -2.7159999 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     5.3323894838800010    0.0000000000000000    0.0000000000000000
    -2.6661947419399987    4.6179847559130724    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.2989605531014377
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.7497556000401238  0.1972471678502988  9.0169746245084816   F   F   F
 -1.3389094814876494  2.5473559251754549 10.8612336967246357   F   F   F
  2.4666406160115706  2.8149609390317449 11.6081185941916623   F   F   F
  3.7425240048606119  1.5166063388643334  9.5654178022134708   F   F   F
 -0.6737595380705244  4.0399616182981788 10.2987723773365900   F   F   F
  1.1865395262746576  3.6893348430173525  8.2518078419286844   F   F   F
 -0.2095461174531081  1.8454906592881426 11.9218080039603862   F   F   F
  2.8013537776218964 -0.0481665105361378 14.5050718430130097   F   F   F
  1.3121618992419066  2.1602122574511333 12.6701466762358947   F   F   F
 -1.2476452889986622  2.3345691932510810 16.2083920853456398   T   T   T
  2.7505086569802928  2.5796663264396886 17.1142649550899257   T   T   T
  3.7344270449053845  1.0894229187115483 15.1960659655248485   T   T   T
  1.8658079062387156  0.6457308122245325 13.2917821082657603   F   F   F
 -0.8896416591163284  3.7749626082998109 15.5093462968256297   T   T   T
  1.1360346434366904  3.3037883716192287 13.8903255655927005   F   F   F
  0.0743769646433166  1.8782236437100546 17.0578886046084968   T   T   T
  0.0035561016254748  4.5301787880046591 19.6927746717804730   T   T   T
  1.3904679985176733  2.2589756639265461 17.9535698126640355   T   T   T
  4.5457222453613833  2.0142049605872661 21.2381275750520722   T   T   T
  3.5880791031521961  0.8574594017079140 20.6557589045968975   T   T   T
  1.6887303530581492  0.9325157862512716 18.8705842337027647   T   T   T
 -0.9607701570395724  3.4316229634926314 20.4500072036908520   T   T   T
  1.0219367433143980  3.6354000011236964 18.7672863094887710   T   T   T
  0.7440954412504207  1.6279471446033176 21.7072013835710820   T   T   T
  4.9465428905284323  2.0128726372061796 22.8266224532852071   T   T   T
  1.4800642679330018  0.7309752878695637  8.0000000000000000   F   F   F
  1.2642171931581458  1.7751671191497465  8.0158744918591047   F   F   F
```

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  2.1205595935037325  4.1247050274958426  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_2x2/Ru E_tot= -144.93100265 eV
 D3-zero damping= -6.2930437 eV, D3-BJ damping= -7.494306 eV
Ru
 1.0000000000000000
     5.3323894838800010    0.0000000000000000    0.0000000000000000
    -2.6661947419399987    4.6179847559130724    0.0000000000000000
     0.0000000000000014    0.0000000000000024   22.4670451429117826
  16
Cartesian
  6.8851514712090225 -1.0103150853688549  8.0508662805144908
  5.5555792952117873 -0.2424481360357814 10.1506216257395447
  5.5445653691990779 -1.7723920580552288 12.3682301070343765
  6.8794373013388359 -1.0028469911259867 14.4668249616714846
  4.2188589833352879 -1.0092468645174162  8.0509456861868856
  2.8901290255250767 -0.2424523175962737 10.1493459649809150
  2.8774622625988404 -1.7721730464289756 12.3680342791609572
  4.2132487838487602 -1.0026613677204486 14.4660285279625338
  5.5524974513183389  1.2987498829244100  8.0514270262311225
  4.2231904713326784  2.0665835802803256 10.1496965672899044
  4.2103668323055770  0.5373774065156219 12.3678207547469619
  5.5460734316973923  1.3060208706813494 14.4659826074035287
  2.8856573192336681  1.2988814709894962  8.0510971043858870
  1.5563439997553414  2.0673533926649243 10.1514532278715688
  1.5449854950434747  0.5370768224794696 12.3678456351836292
  2.8799196819389770  1.3063019085679199 14.4670887048958985

Interface: O-a-SiO2(0001)/fcc(111)_sqrt3/Au E_tot= -254.31456361 eV
 D3-zero damping= -8.8843027 eV, D3-BJ damping= -9.7850203 eV
Si  O Si  O Si  O  H Au
 1.0000000000000000
     5.0207852410612288    0.0000000000000000    0.0000000000000000
    -2.5103926205306131    4.3481275657050009    0.0000000000000000
     0.0000000000000024    0.0000000000000042   39.6937219539651664
   2   5   3   6   3   7   2  12
Selective dynamics
Cartesian
  2.5890705048726717  0.1857208053120887  9.0169746245084834   F   F   F
 -1.2606687834960508  2.3984982851523862 10.8612336967246375   F   F   F
  2.3224996668588749  2.6504654957369391 11.6081185941916676   F   F   F
  3.5238253591050666  1.4279817229572251  9.5654178022134726   F   F   F
 -0.6343876333480609  3.8038818673924530 10.2987723773365918   F   F   F
  1.1172027398720381  3.4737443664141985  8.2518078419286898   F   F   F
 -0.1973010518100266  1.7376473141508393 11.9218080039603880   F   F   F
  2.6376534842764410 -0.0453518457240104 14.5050718430130114   F   F   F
  1.2354842266328521  2.0339777978630278 12.6701466762358965   F   F   F
 -1.3529093365809910  2.2669532945691029 16.3063038453239706   T   T   T
  2.2070695290832063  2.5003228530263399 16.9667120258203639   T   T   T
  3.5888290102109992  1.0808005754001253 15.1885346532213195   T   T   T
  1.7567772996736166  0.6079967979676503 13.2917821082657621   F   F   F
 -0.8820653626219646  3.6622822798260461 15.6100763600055892   T   T   T
  1.0696491672905615  3.1107277414675849 13.8903255655927058   F   F   F
 -0.3031861653895774  1.8429103255177852 17.4698025697527832   T   T   T
 -0.1158121389255461  4.2199061500181649 19.9724337394404756   T   T   T
  1.1420253386881611  2.1641272900824675 18.1444910211387977   T   T   T
  3.5771360689897578  2.1038352932244284 21.8061669252312527   T   T   T
  3.0424849301161756  0.6853964025872079 21.2126198838424358   T   T   T
  1.5634435157121158  0.8533893771187705 18.9910839068091022   T   T   T
 -1.1270849743173674  3.0921405732353255 20.5572529123734355   T   T   T
  1.0474379797988522  3.4667022434893910 19.1179418001234325   T   T   T
 -0.1055787006533947  1.7819964992407145 22.7155431948652726   T   T   T
  2.4290004729479580  2.8021796692457968 22.7546420095449768   T   T   T
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```
  1.3935750294918510  0.6882599157489785  8.0000000000000018   F   F   F
  1.1903412239658357  1.6714332100435891  8.0158744918591101   F   F   F
  1.9966422824214569  3.8836731991140154  8.0308754104330919   F   F   F
 -2.4450140959247308  3.1039551701041330 26.8601998919931688   T   T   T
 -1.7760543169996001  1.6182592413147587 29.2175053458504053   T   T   T
  2.3992950277485781  1.5448244748503734 24.5341669254728494   T   T   T
  0.0600877231194965  1.5961250083169709 26.8293813076544971   T   T   T
  0.7424035910849345  0.1719892918106416 29.2620852295981031   T   T   T
  1.5581949305009419  1.6221356423156077 31.6928817506769285   T   T   T
 -0.9666051137185908  0.1659874909102926 31.6711255269301866   T   T   T
  4.9592951077550929  0.1564349013576557 24.3751490749254742   T   T   T
  0.0593688170190810  4.4976389360500333 26.8662562399911060   T   T   T
  0.7304776608038944  3.0608847439332725 29.2234271299612658   T   T   T
 -0.0436962816244804  3.1430495127563871 24.4418998508515024   T   T   T
 -0.9524946812982394  3.0550484760911054 31.6936904172225944   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Au E_tot= -221.10461094 eV
 D3-zero damping= -2.20129 eV, D3-BJ damping= -3.1316043 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     5.0207852410612288    0.0000000000000000    0.0000000000000000
    -2.5103926205306131    4.3481275657050018    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.8292737882210872
   2   5   3   6   3   7   4
Selective dynamics
Cartesian
  2.5890705048726712  0.1857208053120888  9.0169746245084816   F   F   F
 -1.2606687834960506  2.3984982851523862 10.8612336967246357   F   F   F
  2.3224996668588749  2.6504654957369387 11.6081185941916658   F   F   F
  3.5238253591050661  1.4279817229572249  9.5654178022134708   F   F   F
 -0.6343876333480609  3.8038818673924530 10.2987723773365900   F   F   F
  1.1172027398720381  3.4737443664141989  8.2518078419286880   F   F   F
 -0.1973010518100266  1.7376473141508393 11.9218080039603862   F   F   F
  2.6376534842764410 -0.0453518457240104 14.5050718430130097   F   F   F
  1.2354842266328521  2.0339777978630278 12.6701466762358947   F   F   F
 -1.3468804577500368  2.2646467172602756 16.3094726166758548   T   T   T
  2.2228404918889426  2.5007647056459819 16.9938607178352825   T   T   T
  3.5842801455210904  1.0844642394094848 15.1883176062854321   T   T   T
  1.7567772996736166  0.6079967979676505 13.2917821082657603   F   F   F
 -0.8756903584890025  3.6615157715561084 15.6181852137631321   T   T   T
  1.0696491672905615  3.1107277414675849 13.8903255655927040   F   F   F
 -0.2916467783548017  1.8201095821128295 17.4607842131291306   T   T   T
 -0.1617328904704101  4.1217387045485196 19.9650500352106022   T   T   T
  1.1542597189202064  2.1001820926304626 18.1478829164263367   T   T   T
  3.5067980783912436  2.0216261292656648 21.8051446991723417   T   T   T
  2.9073499119819388  0.6206274098746277 21.2309540642773023   T   T   T
  1.5770465850329580  0.7385098974524396 18.9176074239946281   T   T   T
 -1.1821634720771270  3.0069965073542870 20.5539520289394027   T   T   T
  1.0488908430660588  3.3497055947533223 19.1932373640931395   T   T   T
 -0.1067627264926674  1.6486713768402854 22.5969528175287486   T   T   T
  2.4514848686730510  2.7780601756002627 22.7993616980613076   T   T   T
  1.3935750294918510  0.6882599157489785  8.0000000000000000   F   F   F
  1.1903412239658355  1.6714332100435894  8.0158744918591065   F   F   F
  1.9966422824214565  3.8836731991140154  8.0308754104330884   F   F   F
  1.5167093760400827  2.4483350344721853 22.7874588106310441   T   T   T
 -0.0317528080163076  0.6969988151034664 22.8292156167925171   T   T   T

Oxidized reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Au E_tot= -208.55082691
eV
 D3-zero damping= -2.0949849 eV, D3-BJ damping= -3.0190549 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     5.0207852410612288    0.0000000000000000    0.0000000000000000
```

```
    -2.5103926205306131    4.3481275657050018    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.4186522310609178
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.5890705048726712  0.1857208053120888  9.0169746245084816   F   F   F
 -1.2606687834960506  2.3984982851523862 10.8612336967246357   F   F   F
  2.3224996668588749  2.6504654957369387 11.6081185941916658   F   F   F
  3.5238253591050661  1.4279817229572249  9.5654178022134708   F   F   F
 -0.6343876333480609  3.8038818673924530 10.2987723773365900   F   F   F
  1.1172027398720381  3.4737443664141989  8.2518078419286880   F   F   F
 -0.1973010518100266  1.7376473141508393 11.9218080039603862   F   F   F
  2.6376534842764410 -0.0453518457240104 14.5050718430130097   F   F   F
  1.2354842266328521  2.0339777978630278 12.6701466762358947   F   F   F
 -1.3064998572602600  2.2553538826003563 16.3176003137842081   T   T   T
  2.3142141565333167  2.5099186568510174 17.0856443746406086   T   T   T
  3.5732124525786162  1.0878838960401187 15.1948725458171339   T   T   T
  1.7567772996736166  0.6079967979676505 13.2917821082657603   F   F   F
 -0.8669722018904882  3.6604575239343857 15.6236755165188068   T   T   T
  1.0696491672905615  3.1107277414675849 13.8903255655927040   F   F   F
 -0.1967554200111915  1.7849376208343417 17.4053274892644048   T   T   T
 -0.0692313273540806  4.4564278955490666 20.0104544170622134   T   T   T
  1.1337880392167705  2.3129623947538303 18.1689837275756503   T   T   T
  4.2480180619438919  2.0424481181227008 21.6746164802009069   T   T   T
  3.3979208460420476  0.7948328775216823 21.1257724115327470   T   T   T
  1.4831735875964327  1.2206677771187127 19.3205864498217466   T   T   T
 -1.0228152228784992  3.3161322605843138 20.6937267504087572   T   T   T
  0.8552863015480304  3.7561415677898498 18.8678348749512530   T   T   T
  0.7489295813007473  1.7995556383992537 22.2498537246121408   T   T   T
  4.5613568639396993  2.2311290632112777 23.2689613898249128   T   T   T
  1.3935750294918510  0.6882599157489785  8.0000000000000000   F   F   F
  1.1903412239658355  1.6714332100435894  8.0158744918591065   F   F   F
  1.9966422824214565  3.8836731991140154  8.0308754104330884   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Au E_tot= -42.63862553 eV
 D3-zero damping= -5.8784015 eV, D3-BJ damping= -5.9395813 eV
Au
 1.0000000000000000
     5.0207852410612288    0.0000000000000000    0.0000000000000000
     2.5103926205306144    4.3481275657049991    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.1884510584595631
  12
Cartesian
  5.8572745733696729  1.4489731533193795 10.4154035471762718
  5.8580695118352253  4.3481740138940355 10.4154008366834887
  5.0209994683246419  2.8985367092034440 15.1880813685493834
  2.5102449548892651  1.4495294813966610  8.0005703946064095
  3.3469029458735742  2.8992267377854590 10.4153823755358381
  1.6739143499707458  2.8991627297500533 12.7737862987038557
  2.5105896790493381  1.4491627390196555 15.1880503855233417
  5.0206404168980754  0.0001547458663685  8.0000000000000000
  2.5106252086037273  4.3478713868465828 15.1884510584595596
  4.1842835749623841  1.4488850053799252 12.7737940005022423
  5.0206393097978870  2.8989057635229751  8.0005704382453189
  4.1834916192185432  4.3480784790973770 12.7737862340784716

Interface: O-a-SiO2(0001)/fcc(111)_sqrt3/Ag E_tot= -247.64411455 eV
 D3-zero damping= -7.3129692 eV, D3-BJ damping= -9.3213918 eV
Si  O Si  O Si  O  H Ag
 1.0000000000000000
     4.9892192065539964    0.0000000000000000    0.0000000000000000
    -2.4946096032769969    4.3207905779250027    0.0000000000000000
     0.0000000000000024    0.0000000000000042   39.4405769885361366
```

```
   2   5   3   6   3   7   2  12
Selective dynamics
Cartesian
  2.5727928341549342  0.1845531653777519  9.0169746245084816   F   F   F
 -1.2527428690401645  2.3834187555570008 10.8612336967246357   F   F   F
  2.3078979459910838  2.6338018303376645 11.6081185941916658   F   F   F
  3.5016708180238667  1.4190039001310417  9.5654178022134708   F   F   F
 -0.6303991931014126  3.7799665910915370 10.2987723773365900   F   F   F
  1.1101788066533926  3.4519046881019761  8.2518078419286880   F   F   F
 -0.1960606060409436  1.7267226016912620 11.9218080039603862   F   F   F
  2.6210703689059867 -0.0450667154389341 14.5050718430130097   F   F   F
  1.2277166492801925  2.0211900345408274 12.6701466762358947   F   F   F
 -1.3552014448747085  2.2579841322242409 16.3172206284468473   T   T   T
  2.1741140717181144  2.4837583476098413 16.9823965082673567   T   T   T
  3.5695817537673227  1.0840244860220565 15.1858741871212413   T   T   T
  1.7457323156321762  0.6041742787832056 13.2917821082657603   F   F   F
 -0.8826753484551014  3.6514028460815138 15.6193552930624779   T   T   T
  1.0629242067706033  3.0911703745388581 13.8903255655927040   F   F   F
 -0.3221190829386774  1.8259585969106604 17.4890771872811150   T   T   T
 -0.1783969975991948  4.1017388006905637 19.9849456836105581   T   T   T
  1.1282195658793055  2.1083945578589254 18.1668788217040742   T   T   T
  3.4780241573773019  2.0182769057328547 21.8129153010266137   T   T   T
  2.8286921802943876  0.6150526144482829 21.2790256801145787   T   T   T
  1.5369418312393015  0.7539641133950761 18.9512857518698397   T   T   T
 -1.1731114598906152  2.9274934539669037 20.5068786161441103   T   T   T
  1.0487941535028378  3.3766851002837450 19.1916776926294474   T   T   T
 -0.2043053101805326  1.6363117969138563 22.7305440887011905   T   T   T
  2.4352148288677591  2.8232530962624756 22.7922715150127466   T   T   T
  1.3848135239987263  0.6839327766248433  8.0000000000000000   F   F   F
  1.1828574638870746  1.6609247903738371  8.0158744918591047   F   F   F
  1.9840892501447380  3.8592562690259773  8.0308754104330866   F   F   F
 -2.6197005377050839  2.9886603759649772 26.7124739868084511   T   T   T
 -1.7731341884030849  1.5322847258910819 29.0554036238103421   T   T   T
  1.5210608116103246  1.4956113649280425 24.3530874165059394   T   T   T
 -0.1025880381014894  1.5226736992577250 26.7203871878913226   T   T   T
  0.7263791176543624  0.0920009118857926 29.0653160783080509   T   T   T
  1.5517007635804438  1.5274919681754158 31.4395692841657528   T   T   T
 -0.9422285835022542  0.0857826637494843 31.4405769885361366   T   T   T
  4.0394239072094802  0.0736858274651186 24.2769935911419985   T   T   T
 -0.0963340909210658  4.4353377474455646 26.7076170052590030   T   T   T
  0.7205133510213465  2.9767788859832667 29.0612479099716907   T   T   T
 -0.9075834252182182  3.0246141835813942 24.4646573355020074   T   T   T
 -0.9450192286874924  2.9609117009428112 31.4377587184613461   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Ag E_tot= -221.21160952 eV
 D3-zero damping= -2.2322003 eV, D3-BJ damping= -3.1742167 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.9892192065539955    0.0000000000000000    0.0000000000000000
    -2.4946096032769964    4.3207905779250009    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.8308957786443720
   2   5   3   6   3   7   4
Selective dynamics
Cartesian
  2.5727928341549338  0.1845531653777518  9.0169746245084816   F   F   F
 -1.2527428690401643  2.3834187555570003 10.8612336967246357   F   F   F
  2.3078979459910833  2.6338018303376636 11.6081185941916658   F   F   F
  3.5016708180238663  1.4190039001310413  9.5654178022134708   F   F   F
 -0.6303991931014125  3.7799665910915357 10.2987723773365900   F   F   F
  1.1101788066533924  3.4519046881019753  8.2518078419286880   F   F   F
 -0.1960606060409436  1.7267226016912613 11.9218080039603862   F   F   F
  2.6210703689059862 -0.0450667154389341 14.5050718430130097   F   F   F
  1.2277166492801923  2.0211900345408269 12.6701466762358947   F   F   F
```

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 -1.3539367185918179  2.2559838577824509 16.3147359554581328   T   T   T
  2.1736456487186668  2.4836778118089731 16.9786957029326437   T   T   T
  3.5718167462991346  1.0832470909472720 15.1853683440197713   T   T   T
  1.7457323156321760  0.6041742787832056 13.2917821082657603   F   F   F
 -0.8764399959330161  3.6522897029096630 15.6282573917342162   T   T   T
  1.0629242067706028  3.0911703745388572 13.8903255655927040   F   F   F
 -0.3248880194812049  1.8147722803086044 17.4904201607770133   T   T   T
 -0.1705339251551568  4.0909697972526988 19.9809248249440721   T   T   T
  1.1306702077662425  2.0900513955241533 18.1580006775501488   T   T   T
  3.4786636144150820  2.0009913318924273 21.8252416659736710   T   T   T
  2.8572727159821847  0.6028637211541720 21.2676523151290802   T   T   T
  1.5555497243038314  0.7321095065488236 18.9306652484236650   T   T   T
 -1.1813158120567002  2.9596769989336265 20.5533851755663726   T   T   T
  1.0500694402772208  3.3394548387082903 19.2055170009445746   T   T   T
 -0.1056930950783753  1.6201162069567145 22.6150092339965312   T   T   T
  2.4354881754519928  2.7846793978388407 22.8129744750288310   T   T   T
  1.3848135239987260  0.6839327766248431  8.0000000000000000   F   F   F
  1.1828574638870744  1.6609247903738367  8.0158744918591065   F   F   F
  1.9840892501447374  3.8592562690259764  8.0308754104330884   F   F   F
  1.5034394107015359  2.4455169592123505 22.8146254568939071   T   T   T
 -0.0263032944873756  0.6631280069862723 22.8292530617936400   T   T   T

Oxidized reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Ag E_tot= -208.64710264
eV
 D3-zero damping= -2.1223704 eV, D3-BJ damping= -3.0561732 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.9892192065539955    0.0000000000000000    0.0000000000000000
    -2.4946096032769964    4.3207905779250009    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.4186522310609178
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.5727928341549338  0.1845531653777518  9.0169746245084816   F   F   F
 -1.2527428690401643  2.3834187555570003 10.8612336967246357   F   F   F
  2.3078979459910833  2.6338018303376636 11.6081185941916658   F   F   F
  3.5016708180238663  1.4190039001310413  9.5654178022134708   F   F   F
 -0.6303991931014125  3.7799665910915357 10.2987723773365900   F   F   F
  1.1101788066533924  3.4519046881019753  8.2518078419286880   F   F   F
 -0.1960606060409436  1.7267226016912613 11.9218080039603862   F   F   F
  2.6210703689059862 -0.0450667154389341 14.5050718430130097   F   F   F
  1.2277166492801923  2.0211900345408269 12.6701466762358947   F   F   F
 -1.3085541722315222  2.2445315649230859 16.3257890669532024   T   T   T
  2.2726461756028322  2.4920820485134700 17.0794249790881132   T   T   T
  3.5605806710954524  1.0870550296144246 15.1918427291118547   T   T   T
  1.7457323156321760  0.6041742787832056 13.2917821082657603   F   F   F
 -0.8643179322288002  3.6495137636217221 15.6358200376933159   T   T   T
  1.0629242067706028  3.0911703745388572 13.8903255655927040   F   F   F
 -0.2229714358488850  1.7754885383880690 17.4366661661448141   T   T   T
 -0.0792558804518141  4.4234178146517857 20.0348111912283393   T   T   T
  1.1145669644540666  2.3023501145096836 18.1863335088584464   T   T   T
  4.2042537616691282  2.0240420275803435 21.7086248614943074   T   T   T
  3.3594792952165888  0.7664432551340749 21.1746161589715136   T   T   T
  1.4634408697693346  1.2194619359611487 19.3461413090011405   T   T   T
 -1.0363561760954476  3.2750874788888047 20.6990155814809960   T   T   T
  0.8534003619574869  3.7470844381110897 18.8859225959095625   T   T   T
  0.7349906390673989  1.7975345223623900 22.2941334354616352   T   T   T
  4.5097260274525173  2.2416386249776972 23.3008249755726986   T   T   T
  1.3848135239987260  0.6839327766248431  8.0000000000000000   F   F   F
  1.1828574638870744  1.6609247903738367  8.0158744918591065   F   F   F
  1.9840892501447374  3.8592562690259764  8.0308754104330884   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Ag E_tot= -34.93293542 eV
```

```
 D3-zero damping= -4.3721298 eV, D3-BJ damping= -5.4169809 eV
Ag
 1.0000000000000000
     4.9892192065539964    0.0000000000000000    0.0000000000000000
     2.4946096032769982    4.3207905779250000    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.0795847403917733
  12
Cartesian
  5.8207103770049606  1.4402884322230407 10.3699668397062723
  5.8207421296715482  4.3208250380505557 10.3699653615784406
  4.9893354737130222  2.8803918737569485 15.0795263970611622
  2.4945236448711592  1.4403588282938187  8.0000560297603656
  3.3261123009183318  2.8805715803445779 10.3699658515051176
  1.6631335541781627  2.8804617680119411 12.7102937657415538
  2.4947289682325886  1.4401316754582061 15.0795252626000682
  4.9891266505965275  0.0001020320955719  8.0000000000000000
  2.4947677325361566  4.3206221229474151 15.0795847403917733
  4.1577404951933525  1.4402001477997917 12.7102863423017887
  4.9891330678717347  2.8806229254474403  8.0000595444143716
  4.1577428402490870  4.3207255949594137 12.7102958358489708

Interface: O-a-SiO2(0001)/fcc(111)_sqrt3/Cu E_tot= -250.3677418 eV
 D3-zero damping= -7.9690679 eV, D3-BJ damping= -10.276596 eV
Si  O Si  O Si  O  H Cu
 1.0000000000000000
     4.3712972374160088    0.0000000000000000    0.0000000000000000
    -2.1856486187080035    3.7856544550950013    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.9617534681092508
   2   5   3   6   3   7   2  12
Selective dynamics
Cartesian
  2.2541487440783290  0.1616959906095912  9.0169746245084816   F   F   F
 -1.0975888642924896  2.0882289172793960 10.8612336967246357   F   F   F
  2.0220614685152176  2.3076016884029165 11.6081185941916658   F   F   F
  3.0679838546801932  1.2432582277357256  9.5654178022134708   F   F   F
 -0.5523233470386633  3.3118122962923007 10.2987723773365900   F   F   F
  0.9726815659225442  3.0243813314720174  8.2518078419286880   F   F   F
 -0.1717782182083825  1.5128655258605359 11.9218080039603862   F   F   F
  2.2964470367669541 -0.0394851379628379 14.5050718430130097   F   F   F
  1.0756621778169735  1.7708627439489648 12.6701466762358947   F   F   F
 -1.3232037742261289  2.0549291718440652 16.4384249355902305   T   T   T
  1.5256416787661713  2.2350873011045653 16.9590457436493764   T   T   T
  3.2842319820582810  1.0745763921460427 15.1667916110094456   T   T   T
  1.5295208594094865  0.5293464260486898 13.2917821082657603   F   F   F
 -0.8508936118600373  3.4537827947598565 15.7888891959609232   T   T   T
  0.9312795161486062  2.7083244810838480 13.8903255655927040   F   F   F
 -0.6621077523541422  1.5797645848691348 17.8448240489595626   T   T   T
 -0.2616965353775919  3.3972727324848875 20.3231468977739951   T   T   T
  0.8612151390491893  1.7773049097687663 18.3774444164006567   T   T   T
  2.8748009718854108  1.5896837637708710 22.2822297195771490   T   T   T
  2.0507046068168462  0.2684834529911951 21.8046482847214769   T   T   T
  1.1927665100597082  0.3969497613667445 19.1233943848564039   T   T   T
 -1.0580142378005255  2.0576333001626406 20.7876703882795617   T   T   T
  1.0711322704179356  2.8883147234262356 19.5537511480221653   T   T   T
 -0.2805682314567331  1.2576838591292194 23.3206343488741012   T   T   T
  1.9455695787587168  2.5181335034719696 23.2436207454636587   T   T   T
  1.2133023788251236  0.5992267193053191  8.0000000000000000   F   F   F
  1.0363588670055190  1.4552168680380753  8.0158744918591083   F   F   F
  1.7383569450208372  3.3812818336610184  8.0308754104330902   F   F   F
 -2.4304439209253514  2.5526325001996235 26.8256189348286895   T   T   T
 -1.6993430803739606  1.2889214586249811 28.8772967743904232   T   T   T
  1.2071250609920239  1.2871667758003253 24.7363676855639767   T   T   T
 -0.2371334083480694  1.2901817067707464 26.8223409574940845   T   T   T
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  0.4916535021934718  0.0303506060836785 28.8810788266082064   T   T   T
  1.2171965231257180  1.2933207482978559 30.9605326870811304   T   T   T
 -0.9663770021722180  0.0300416267008446 30.9612225665987069   T   T   T
  3.4020166091831423 -0.0002926184045598 24.7525345178038627   T   T   T
 -0.2407544854699614  3.8189657288495829 26.7985675327899990   T   T   T
  0.4847657834963672  2.5576043510938802 28.8815098989940182   T   T   T
 -0.9630077391647149  2.5803265272387583 24.7741150212692709   T   T   T
 -0.9694023410150457  2.5513859064342710 30.9609027723987467   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Cu E_tot= -212.01830878 eV
 D3-zero damping= -2.8745065 eV, D3-BJ damping= -4.1576796 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.3712972374160088    0.0000000000000000    0.0000000000000000
    -2.1856486187080035    3.7856544550950013    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.3515305166237823
   2   5   3   6   3   7   4
Selective dynamics
Cartesian
  2.2541487440783290  0.1616959906095912  9.0169746245084816   F   F   F
 -1.0975888642924896  2.0882289172793960 10.8612336967246357   F   F   F
  2.0220614685152176  2.3076016884029165 11.6081185941916658   F   F   F
  3.0679838546801932  1.2432582277357256  9.5654178022134708   F   F   F
 -0.5523233470386633  3.3118122962923007 10.2987723773365900   F   F   F
  0.9726815659225442  3.0243813314720174  8.2518078419286880   F   F   F
 -0.1717782182083825  1.5128655258605359 11.9218080039603862   F   F   F
  2.2964470367669541 -0.0394851379628379 14.5050718430130097   F   F   F
  1.0756621778169735  1.7708627439489648 12.6701466762358947   F   F   F
 -1.3308726410722245  2.0596737827719847 16.4384790933869631   T   T   T
  1.5171623701160279  2.2391638655783113 16.9599704654185288   T   T   T
  3.2822381286104441  1.0717769173858329 15.1749566292750284   T   T   T
  1.5295208594094865  0.5293464260486898 13.2917821082657603   F   F   F
 -0.8576483308496390  3.4557210554600895 15.7857365159086012   T   T   T
  0.9312795161486062  2.7083244810838480 13.8903255655927040   F   F   F
 -0.6729242045897293  1.5961505777288321 17.8511616874765622   T   T   T
 -0.2752894280402552  3.4051497178738463 20.3263857021261778   T   T   T
  0.8510643718477336  1.7929133135400921 18.3804332306644156   T   T   T
  2.8658886573869351  1.5958486619931482 22.2822142554731499   T   T   T
  2.0368348590378296  0.2625338729251592 21.8263251420002682   T   T   T
  1.1756426422308017  0.4186196095744958 19.1408758918333923   T   T   T
 -1.0637172953315319  2.0571361874305065 20.7818588935390878   T   T   T
  1.0596305609099794  2.9127577436577465 19.5503124349414001   T   T   T
 -0.2751026171189622  1.2668649932723255 23.3042054025075451   T   T   T
  1.8792526826425278  2.5651824258311171 23.1335813345182899   T   T   T
  1.2133023788251236  0.5992267193053191  8.0000000000000000   F   F   F
  1.0363588670055190  1.4552168680380753  8.0158744918591065   F   F   F
  1.7383569450208372  3.3812818336610184  8.0308754104330884   F   F   F
  0.9643281508942627  2.1316641580099991 23.2904784618024507   T   T   T
 -0.1321266759949489  0.2560489934729470 23.3516727737666407   T   T   T

Oxidized reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Cu E_tot= -199.40871599
eV
 D3-zero damping= -2.7243838 eV, D3-BJ damping= -3.9698904 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.3712972374160088    0.0000000000000000    0.0000000000000000
    -2.1856486187080035    3.7856544550950013    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.4186522310609178
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.2541487440783290  0.1616959906095912  9.0169746245084816   F   F   F
 -1.0975888642924896  2.0882289172793960 10.8612336967246357   F   F   F
```

```
  2.0220614685152176  2.3076016884029165 11.6081185941916658   F   F   F
  3.0679838546801932  1.2432582277357256  9.5654178022134708   F   F   F
 -0.5523233470386633  3.3118122962923007 10.2987723773365900   F   F   F
  0.9726815659225442  3.0243813314720174  8.2518078419286880   F   F   F
 -0.1717782182083825  1.5128655258605359 11.9218080039603862   F   F   F
  2.2964470367669541 -0.0394851379628379 14.5050718430130097   F   F   F
  1.0756621778169735  1.7708627439489648 12.6701466762358947   F   F   F
 -1.1602207020304598  1.9969613889629960 16.5006763624238957   T   T   T
  1.9742229523917665  2.3831706307924128 17.4502940113095910   T   T   T
  3.2270841767437264  1.1457457354532647 15.1210722870528862   T   T   T
  1.5295208594094865  0.5293464260486898 13.2917821082657603   F   F   F
 -0.7175266686976610  3.4250101002795095 15.8686769447237594   T   T   T
  0.9312795161486062  2.7083244810838480 13.8903255655927040   F   F   F
 -0.2055790006137519  1.2703779095048167 17.5862891952755120   T   T   T
 -0.3191387134051685  3.9381194921871652 20.4852019733958457   T   T   T
  0.8167439162215328  2.0900082033477121 18.5174526948107392   T   T   T
  3.5456656190230325  1.7572707671703576 22.3199670764533096   T   T   T
  2.9552406323991796  0.4220536826805793 21.6506218051186785   T   T   T
  0.9790033279278979  1.4211862451882298 20.0040336452686880   T   T   T
 -1.2751170844548312  2.8577510443489200 21.2102973903376579   T   T   T
  0.2462263867035076  3.5270371516598367 19.0161206567790515   T   T   T
  0.6698998997430505  1.6358816614008513 22.9970925086495299   T   T   T
  3.7501689521417134  2.0415139511685476 23.9162052502787468   T   T   T
  1.2133023788251236  0.5992267193053191  8.0000000000000000   F   F   F
  1.0363588670055190  1.4552168680380753  8.0158744918591065   F   F   F
  1.7383569450208372  3.3812818336610184  8.0308754104330884   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Cu E_tot= -46.32239467 eV
 D3-zero damping= -4.3621417 eV, D3-BJ damping= -5.3255084 eV
Cu
 1.0000000000000000
     4.3712972374160088    0.0000000000000000    0.0000000000000000
     2.1856486187080044    3.7856544550949991    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.1910562705090015
  12
Cartesian
  5.0998395037423112  1.2618881788428995 10.0692388600749183
  5.0998394815583401  3.7856577222838950 10.0692388369305323
  4.3713715760769913  2.5236955363934421 14.1910562705089980
  2.1856126228030477  1.2619174447456631  8.0000000599177330
  2.9141908829507575  2.5237729685808548 10.0692388040251863
  1.4571309268965353  2.5237401457261202 12.1219743229249115
  2.1857229184353835  1.2618107213504677 14.1910561280621899
  4.3712611973561959  0.0000326417149119  8.0000001557311613
  2.1857229844484767  3.7855804354035851 14.1910561453164430
  3.6427795892181440  1.2618553396925982 12.1219742618574671
  4.3712612470000343  2.5238022950423686  8.0000000000000000
  3.6427796691557450  3.7856249270563578 12.1219742822319443

Interface: O-a-SiO2(0001)/fcc(111)_sqrt3/Pt E_tot= -288.25665085 eV
 D3-zero damping= -9.9229729 eV, D3-BJ damping= -11.1607178 eV
Si  O Si  O Si  O  H Pt
 1.0000000000000000
     4.7985659889076251    0.0000000000000000    0.0000000000000000
    -2.3992829944538112    4.1556800481300007    0.0000000000000000
     0.0000000000000024    0.0000000000000042   39.6024486534592910
   2   5   3   6   3   7   2  12
Selective dynamics
Cartesian
  2.4744786066451843  0.1775008284590071  9.0169746245084816   F   F   F
 -1.2048717595582827  2.2923410867007736 10.8612336967246357   F   F   F
  2.2197061566175798  2.5331562638055005 11.6081185941916658   F   F   F
  3.3678613418401659  1.3647794517329139  9.5654178022134708   F   F   F
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 -0.6063097254731756  3.6355225882622553 10.2987723773365900   F   F   F
  1.0677555029482286  3.3199969268773910  8.2518078419286880   F   F   F
 -0.1885685348675022  1.6607392871953384 11.9218080039603862   F   F   F
  2.5209113101793137 -0.0433445793788669 14.5050718430130097   F   F   F
  1.1808018676574870  1.9439542251673312 12.6701466762358947   F   F   F
 -1.3617707963741643  2.1930450377767765 16.3514890160351243   T   T   T
  1.9411800230995975  2.3784400465465474 16.9446336507353017   T   T   T
  3.4916309829652832  1.0807059949791404 15.1673437129254722   T   T   T
  1.6790225822359550  0.5810869447735314 13.2917821082657603   F   F   F
 -0.8681055655546087  3.5896757274616218 15.6873876169273476   T   T   T
  1.0223066448344940  2.9730473669498561 13.8903255655927040   F   F   F
 -0.4611014922237949  1.7468953871895592 17.6222481897563483   T   T   T
 -0.2342270765416964  3.8259504648756013 20.0687537642045513   T   T   T
  1.0286840141010247  1.9715321290746479 18.2248226383731726   T   T   T
  3.2410612725003394  1.8372180037121648 21.9048364350500044   T   T   T
  2.5204333424530914  0.4520023192177574 21.4458809699573365   T   T   T
  1.4311781418167533  0.5959675451127120 18.9665113435566894   T   T   T
 -1.1912730506016165  2.5882199516822526 20.5132500262306898   T   T   T
  1.0607445136051723  3.1810082023811317 19.3217737345281009   T   T   T
 -0.1961194342725072  1.4926807585454842 22.7552101118093510   T   T   T
  2.2322689360210490  2.8018318933681683 22.7654397275985971   T   T   T
  1.3318955937053962  0.6577976281939918  8.0000000000000000   F   F   F
  1.1376568879711371  1.5974558100697802  8.0158744918591047   F   F   F
  1.9082711744144194  3.7117823668079328  8.0308754104330866   F   F   F
 -1.8482727451909353  4.1181843045847417 27.0093328095739125   T   T   T
 -1.0420905426166895  2.7059519991502494 29.2774171601098381   T   T   T
  2.1812838626886433  2.7855043592490349 24.7340408294596159   T   T   T
  0.5724580537065839  2.7208800819797312 27.0119917745457947   T   T   T
  1.3539232284331868  1.3280677580249616 29.2754976549869248   T   T   T
  2.1494592166018101  2.6892271683911320 31.6001835243206699   T   T   T
 -0.2453663000844671  1.3007074994065897 31.5997572465590544   T   T   T
  4.5903191213729713  1.3960243290993390 24.7270560224095242   T   T   T
  0.5716483595199421  5.5107490300715583 27.0432858119427522   T   T   T
  1.3649372311956416  4.0922031449270033 29.2758793879316670   T   T   T
 -0.2129830661481170  4.1700269910286609 24.8008124731147888   T   T   T
 -0.2487724567060386  4.0714933819236530 31.5693462917639529   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Pt E_tot= -220.6185139 eV
 D3-zero damping= -2.4223994 eV, D3-BJ damping= -3.4443539 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.7985659889076251    0.0000000000000000    0.0000000000000000
    -2.3992829944538112    4.1556800481300007    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.9653861426206127
   2   5   3   6   3   7   4
Selective dynamics
Cartesian
  2.4744786066451843  0.1775008284590071  9.0169746245084816   F   F   F
 -1.2048717595582827  2.2923410867007736 10.8612336967246357   F   F   F
  2.2197061566175798  2.5331562638055005 11.6081185941916658   F   F   F
  3.3678613418401659  1.3647794517329139  9.5654178022134708   F   F   F
 -0.6063097254731756  3.6355225882622553 10.2987723773365900   F   F   F
  1.0677555029482286  3.3199969268773910  8.2518078419286880   F   F   F
 -0.1885685348675022  1.6607392871953384 11.9218080039603862   F   F   F
  2.5209113101793137 -0.0433445793788669 14.5050718430130097   F   F   F
  1.1808018676574870  1.9439542251673312 12.6701466762358947   F   F   F
 -1.3695934052727046  2.1991520481669546 16.3526214003785348   T   T   T
  1.9280524456066130  2.3844669836153587 16.9341864000503328   T   T   T
  3.4916245938655819  1.0741879912346755 15.1813468417460911   T   T   T
  1.6790225822359550  0.5810869447735314 13.2917821082657603   F   F   F
 -0.8744874855427480  3.5911080582795778 15.6829294460378446   T   T   T
  1.0223066448344940  2.9730473669498561 13.8903255655927040   F   F   F
 -0.4759449241864004  1.7795985834547488 17.6393327935592801   T   T   T
```

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 -0.2097523784094658  3.8910032623046611 20.0809529791249020   T   T   T
  1.0183214147037307  2.0169229649076499 18.2271729205054100   T   T   T
  3.3050097493286339  1.8723029380999072 21.9555478243173852   T   T   T
  2.5955450394507960  0.4924699311974089 21.4607354407351743   T   T   T
  1.4200927401504448  0.6660144101715232 19.0116154606226679   T   T   T
 -1.1581079593780523  2.6773345291287902 20.5839563211037913   T   T   T
  1.0629968218772297  3.2518190769179021 19.2935232514398578   T   T   T
 -0.1266048086647125  1.4752220856012308 22.7847782098235605   T   T   T
  2.3071680805784753  2.7661711875961221 22.9023513278419699   T   T   T
  1.3318955937053962  0.6577976281939918  8.0000000000000000   F   F   F
  1.1376568879711371  1.5974558100697802  8.0158744918591065   F   F   F
  1.9082711744144194  3.7117823668079328  8.0308754104330884   F   F   F
  1.3832490637054493  2.3986609731370709 22.9653934283349024   T   T   T
 -0.0239824630759832  0.4967612908647248 22.9222153915774989   T   T   T

Oxidized reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Pt E_tot= -207.98021131
eV
 D3-zero damping= -2.2970812 eV, D3-BJ damping= -3.30266 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.7985659889076251    0.0000000000000000    0.0000000000000000
    -2.3992829944538112    4.1556800481300007    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.4186522310609178
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.4744786066451843  0.1775008284590071  9.0169746245084816   F   F   F
 -1.2048717595582827  2.2923410867007736 10.8612336967246357   F   F   F
  2.2197061566175798  2.5331562638055005 11.6081185941916658   F   F   F
  3.3678613418401659  1.3647794517329139  9.5654178022134708   F   F   F
 -0.6063097254731756  3.6355225882622553 10.2987723773365900   F   F   F
  1.0677555029482286  3.3199969268773910  8.2518078419286880   F   F   F
 -0.1885685348675022  1.6607392871953384 11.9218080039603862   F   F   F
  2.5209113101793137 -0.0433445793788669 14.5050718430130097   F   F   F
  1.1808018676574870  1.9439542251673312 12.6701466762358947   F   F   F
 -1.3091153948012981  2.1799102298482631 16.3713742499027184   T   T   T
  2.0566358025422575  2.4161169814058452 17.0718326766462525   T   T   T
  3.4764357818244798  1.0879910970336306 15.1746832822049669   T   T   T
  1.6790225822359550  0.5810869447735314 13.2917821082657603   F   F   F
 -0.8427707711498811  3.5847198107711140 15.7044956618527092   T   T   T
  1.0223066448344940  2.9730473669498561 13.8903255655927040   F   F   F
 -0.3383084420017706  1.6893526891309278 17.5720153876771477   T   T   T
 -0.1029921979893235  4.3104406910714426 20.1714286537043748   T   T   T
  0.9973030813307429  2.2643559458212694 18.2767807235555857   T   T   T
  4.0486803548736754  1.9792300573166655 21.8945493768300281   T   T   T
  3.2656725107766356  0.6858275531154056 21.3553693283229009   T   T   T
  1.3522684592899972  1.3034012596581226 19.5358434081421777   T   T   T
 -1.0593139196233419  3.1613053981145485 20.8217715217640027   T   T   T
  0.7615319884930970  3.7280667588368690 18.9297818408198246   T   T   T
  0.7668919187289844  1.8111806975970950 22.5073057996732544   T   T   T
  4.3249902943548824  2.2553176447084349 23.4816894251462216   T   T   T
  1.3318955937053962  0.6577976281939918  8.0000000000000000   F   F   F
  1.1376568879711371  1.5974558100697802  8.0158744918591065   F   F   F
  1.9082711744144194  3.7117823668079328  8.0308754104330884   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Pt E_tot= -76.27530903 eV
 D3-zero damping= -6.656523 eV, D3-BJ damping= -6.9253747 eV
Pt
 1.0000000000000000
     4.7985659889076251    0.0000000000000000    0.0000000000000000
     2.3992829944538125    4.1556800481299989    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.8578987326980325
  12
```

```
Cartesian
  5.5983072969349434  1.3852552135053127 10.2998504961580259
  5.5983074313317642  4.1557085677605325 10.2998504960837671
  4.7982295282700358  2.7705754626834769 14.8578987326980325
  2.3997061748454844  1.3850260679897639  8.0000000924258732
  3.1990242999908638  2.7704820195253261 10.2998506747447713
  1.5995237438406782  2.7704292760624218 12.5569129382707025
  2.3989465070371874  1.3853489325836321 14.8578986958401522
  4.7989891555223521 -0.0002006601011906  8.0000000260745274
  2.3989465337284495  4.1558020361918420 14.8578985860271295
  3.9988067642492564  1.3852026030788183 12.5569129227630683
  4.7989891692992996  2.7702525991105218  8.0000000000000000
  3.9988067717429701  4.1556559493417504 12.5569129196091431

Interface: O-a-SiO2(0001)/fcc(111)_sqrt3/Pd E_tot= -275.89867742 eV
 D3-zero damping= -8.2416519 eV, D3-BJ damping= -10.2901542 eV
Si  O Si  O Si  O  H Pd
 1.0000000000000000
     4.7596431118965139    0.0000000000000000    0.0000000000000000
    -2.3798215559482556    4.1219718478500011    0.0000000000000000
     0.0000000000000024    0.0000000000000042   39.3572266685787540
   2   5   3   6   3   7   2  12
Selective dynamics
Cartesian
  2.4544072297597319  0.1760610560496143  9.0169746245084816   F   F   F
 -1.1950986157857773  2.2737470920800007 10.8612336967246357   F   F   F
  2.2017013297725287  2.5126089315537516 11.6081185941916658   F   F   F
  3.3405434195479762  1.3537092397425221  9.5654178022134708   F   F   F
 -0.6013917314454212  3.6060335703137372 10.2987723773365900   F   F   F
  1.0590945579460631  3.2930672498945532  8.2518078419286880   F   F   F
 -0.1870389883513597  1.6472684396186983 11.9218080039603862   F   F   F
  2.5004633011055932 -0.0429929960649848 14.5050718430130097   F   F   F
  1.1712239633469981  1.9281861204051327 12.6701466762358947   F   F   F
 -1.3636221905357877  2.1843998737701642 16.3593186094614857   T   T   T
  1.8922080645103136  2.3708473126246021 16.9319648766255852   T   T   T
  3.4733147053386539  1.0800520920790124 15.1695798314628210   T   T   T
  1.6654034323444422  0.5763735416992661 13.2917821082657603   F   F   F
 -0.8658413719939361  3.5801758983695788 15.6999944733835637   T   T   T
  1.0140143517001459  2.9489319213605913 13.8903255655927040   F   F   F
 -0.4913802455454012  1.7466995628530071 17.6547477408388005   T   T   T
 -0.2014591095578978  3.8469901501060977 20.1066282266670058   T   T   T
  1.0062709990560490  1.9802684004482836 18.2361663525767135   T   T   T
  3.2559178982333603  1.8704510362249713 21.9893161310235747   T   T   T
  2.6123144809010368  0.4735615931101529 21.4734714976835228   T   T   T
  1.4213368645836200  0.6257931210496062 19.0025677333000509   T   T   T
 -1.1893670096982016  2.6663163824169405 20.6136066708798324   T   T   T
  1.0625609475128888  3.1864379292070337 19.3291113580100422   T   T   T
 -0.1597069061750658  1.5802767515641700 22.8906026047295228   T   T   T
  2.1852171991993123  2.6635961036242346 22.9460189057960591   T   T   T
  1.3210921143940202  0.6524619974577303  8.0000000000000000   F   F   F
  1.1284289479503675  1.5844982773048331  8.0158744918591047   F   F   F
  1.8927925075799366  3.6816747786473782  8.0308754104330866   F   F   F
 -1.8670030234535542  2.8693862521703686 26.8291624309572683   T   T   T
 -1.1146816896676484  1.4540076320194684 29.0646876421150857   T   T   T
  2.3158646935213554  1.4300574103233419 24.6711084001221082   T   T   T
  0.5034896412523264  1.4260125169193227 26.8337985578199323   T   T   T
  1.2748855155543386  0.0783423692835548 29.0814590644049069   T   T   T
  2.0556355849042389  1.4502840185713033 31.3571069708406540   T   T   T
 -0.3267053957208381  0.0776307229964751 31.3510058725019682   T   T   T
  4.7583082646192247  0.0881831950317032 24.3895279151167941   T   T   T
  0.5154461550285439  4.1948951377151849 26.8082864872090134   T   T   T
  1.2679841779737189  2.8227159929084267 29.0658652898645791   T   T   T
 -0.0384659310130547  2.8475676229446787 24.6129544257014850   T   T   T
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 -0.3250701617375145  2.8268037526363137 31.3557788962007429   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Pd E_tot= -220.2852392 eV
 D3-zero damping= -2.4626525 eV, D3-BJ damping= -3.5033834 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.7596431118965130    0.0000000000000000    0.0000000000000000
    -2.3798215559482556    4.1219718478500011    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.9903491216151998
   2   5   3   6   3   7   4
Selective dynamics
Cartesian
  2.4544072297597319  0.1760610560496143  9.0169746245084816   F   F   F
 -1.1950986157857773  2.2737470920800011 10.8612336967246357   F   F   F
  2.2017013297725279  2.5126089315537521 11.6081185941916658   F   F   F
  3.3405434195479757  1.3537092397425223  9.5654178022134708   F   F   F
 -0.6013917314454215  3.6060335703137367 10.2987723773365900   F   F   F
  1.0590945579460624  3.2930672498945532  8.2518078419286880   F   F   F
 -0.1870389883513598  1.6472684396186983 11.9218080039603862   F   F   F
  2.5004633011055928 -0.0429929960649848 14.5050718430130097   F   F   F
  1.1712239633469976  1.9281861204051327 12.6701466762358947   F   F   F
 -1.3718130532212744  2.1882958428930621 16.3585674017689833   T   T   T
  1.8818020794296149  2.3667568495758431 16.9276998057814545   T   T   T
  3.4735639953041275  1.0740607060309524 15.1794407800436737   T   T   T
  1.6654034323444418  0.5763735416992661 13.2917821082657603   F   F   F
 -0.8755860149447043  3.5802790683834078 15.6924122547745846   T   T   T
  1.0140143517001454  2.9489319213605913 13.8903255655927040   F   F   F
 -0.5025558895837715  1.7704578982567849 17.6623600600784201   T   T   T
 -0.2136547528909135  3.8545316598875781 20.1006277580213109   T   T   T
  0.9962384938845599  2.0035408186013890 18.2390582896703783   T   T   T
  3.2785460281487113  1.8476208126021203 21.9817098269825486   T   T   T
  2.5564068018352772  0.4709687334303824 21.4959124849465866   T   T   T
  1.3910644325728534  0.6564059485299689 19.0311169459652909   T   T   T
 -1.1481349716254379  2.6262588398673379 20.5943082972167737   T   T   T
  1.0639735378546940  3.2372957521402146 19.3050824045701859   T   T   T
 -0.1194869401957765  1.4537943323068652 22.8172573669379268   T   T   T
  2.2876939711797744  2.7529804333763850 22.9241674700572950   T   T   T
  1.3210921143940200  0.6524619974577301  8.0000000000000000   F   F   F
  1.1284289479503671  1.5844982773048333  8.0158744918591065   F   F   F
  1.8927925075799359  3.6816747786473782  8.0308754104330884   F   F   F
  1.3633414588145722  2.3837429369011334 22.9904138917673677   T   T   T
 -0.0139916061248492  0.4731637191725329 22.9500449750763984   T   T   T

Oxidized reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Pd E_tot= -207.64286104
eV
 D3-zero damping= -2.3339996 eV, D3-BJ damping= -3.3556437 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.7596431118965130    0.0000000000000000    0.0000000000000000
    -2.3798215559482556    4.1219718478500011    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.4186522310609178
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.4544072297597319  0.1760610560496143  9.0169746245084816   F   F   F
 -1.1950986157857773  2.2737470920800011 10.8612336967246357   F   F   F
  2.2017013297725279  2.5126089315537521 11.6081185941916658   F   F   F
  3.3405434195479757  1.3537092397425223  9.5654178022134708   F   F   F
 -0.6013917314454215  3.6060335703137367 10.2987723773365900   F   F   F
  1.0590945579460624  3.2930672498945532  8.2518078419286880   F   F   F
 -0.1870389883513598  1.6472684396186983 11.9218080039603862   F   F   F
  2.5004633011055928 -0.0429929960649848 14.5050718430130097   F   F   F
  1.1712239633469976  1.9281861204051327 12.6701466762358947   F   F   F
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 -1.3113571488836047  2.1703617565013857 16.3788609659008308   T   T   T
  2.0094577705063532  2.4051989453685669 17.0660157948154740   T   T   T
  3.4577780908172531  1.0891911971898138 15.1729847943511604   T   T   T
  1.6654034323444418  0.5763735416992661 13.2917821082657603   F   F   F
 -0.8402097496189006  3.5743848480344300 15.7163120708684456   T   T   T
  1.0140143517001454  2.9489319213605913 13.8903255655927040   F   F   F
 -0.3658672555291020  1.6836234244414032 17.5998275031166358   T   T   T
 -0.1119458357370140  4.2800371786255749 20.1985273070945155   T   T   T
  0.9752550299744850  2.2562063299101753 18.2932918131448830   T   T   T
  3.9960272959289811  1.9703100311918507 21.9377192111758035   T   T   T
  3.2234170185890356  0.6687089628316161 21.4030940184917711   T   T   T
  1.3269200490515989  1.3051103505131421 19.5597570180198659   T   T   T
 -1.0712270473820544  3.1281473414327778 20.8376316857173727   T   T   T
  0.7584319837515410  3.7184127706226087 18.9528288814800376   T   T   T
  0.7458824502368594  1.8100851060987533 22.5703890339142923   T   T   T
  4.2559206515096406  2.2820901306005008 23.5206440810805084   T   T   T
  1.3210921143940200  0.6524619974577301  8.0000000000000000   F   F   F
  1.1284289479503671  1.5844982773048333  8.0158744918591065   F   F   F
  1.8927925075799359  3.6816747786473782  8.0308754104330884   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Pd E_tot= -64.29714241 eV
 D3-zero damping= -5.0028266 eV, D3-BJ damping= -5.9926421 eV
Pd
 1.0000000000000000
     4.7596431118965139    0.0000000000000000    0.0000000000000000
     2.3798215559482570    4.1219718478499994    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.7848903884610010
  12
Cartesian
  5.5528479283914560  1.3740570459520898 10.2714814415853564
  5.5528478576845748  4.1220382274812941 10.2714814507388983
  4.7598719492758716  2.7477511759738831 14.7899051002088111
  2.3796565062376036  1.3741627216645931  7.9952165569729852
  3.1730263569992152  2.7480476230114292 10.2714814199414946
  1.5866213038474464  2.7478993259487812 12.5134848823296938
  2.3800503095200480  1.3737604481566712 14.7899051261311438
  4.7594781402739592  0.0001719974450671  7.9952167919358681
  2.3800503756470106  4.1217416873580719 14.7899051069846621
  3.9664429230374592  1.3739088333168670 12.5134848944659272
  4.7594779786971992  2.7481532487407856  7.9952165411015388
  3.9664428634001498  4.1218900641908380 12.5134849084948332

Interface: O-a-SiO2(0001)/fcc(111)_sqrt3/Ni E_tot= -264.57677536 eV
 D3-zero damping= -7.0870123 eV, D3-BJ damping= -9.3350578 eV
Si  O Si  O Si  O  H Ni
 1.0000000000000000
     4.2502068721891444    0.0000000000000000    0.0000000000000000
    -2.1251034360945709    3.6807871226550004    0.0000000000000000
     0.0000000000000024    0.0000000000000041   39.0027951514414326
   2   5   3   6   3   7   2  12
Selective dynamics
Cartesian
  2.1917060228742513  0.1572168107471371  9.0169746245084799   F   F   F
 -1.0671842888935668  2.0303823814487334 10.8612336967246339   F   F   F
  1.9660478532346390  2.2436782542207063 11.6081185941916640   F   F   F
  2.9829968896453116  1.2088184299614579  9.5654178022134690   F   F   F
 -0.5370233040116710  3.2200709804448535 10.2987723773365882   F   F   F
  0.9457370778976069  2.9406022105102632  8.2518078419286862   F   F   F
 -0.1670197481133200  1.4709572709156318 11.9218080039603844   F   F   F
  2.2328326002957701 -0.0383913505772471 14.5050718430130079   F   F   F
  1.0458649988794055  1.7218076454770554 12.6701466762358930   F   F   F
 -1.3146735518301833  2.0216621101302383 16.4585254589859815   T   T   T
  1.4196848006728575  2.2429695713255735 16.9896470963950108   T   T   T
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  3.2093986524784359  1.0890163350268434 15.1589297379547503   T   T   T
  1.4871512310294486  0.5146828722841186 13.2917821082657586   F   F   F
 -0.8433515859006118  3.4221086104591603 15.8157070611663979   T   T   T
  0.9054819163483713  2.6333005276083887 13.8903255655927023   F   F   F
 -0.7125894976760353  1.4960147313744709 17.8762068650170072   T   T   T
 -0.3467888809803493  3.2479062846851989 20.3646630727095541   T   T   T
  0.8096766230121186  1.7117156663336555 18.4089354094186533   T   T   T
  2.5568939261783665  1.5640128274902405 22.3232740366057634   T   T   T
  1.6775592444837246  0.2884828085036389 21.8220687783429241   T   T   T
  1.1317288946240351  0.2945201318123548 19.0817188852536255   T   T   T
 -1.0397306904540937  1.8550108788576802 20.8570352994212982   T   T   T
  1.0282659744985077  2.7472479986514857 19.6596273735994522   T   T   T
 -0.5755009357633960  1.2673470352151859 23.4967414090601103   T   T   T
  1.6019689856515604  2.5356821437996562 23.2047997319780350   T   T   T
  1.1796923952886562  0.5826273945846626  7.9999999999999982   F   F   F
  1.0076504386155112  1.4149055525487655  8.0158744918591029   F   F   F
  1.6902022975707685  3.2876161253059846  8.0308754104330848   F   F   F
 -1.2929409582929954  2.5000361913696194 26.8375389162775058   T   T   T
 -0.6042061986283376  1.2640365047384030 28.8537736329049750   T   T   T
  2.2375088528325713  1.2208425758013433 24.9143410132362071   T   T   T
  0.8150715221713294  1.2381634019535535 26.8300037224420684   T   T   T
  1.5237167278682622  0.0380850694565502 28.8495726891401425   T   T   T
  2.2234754474280449  1.2639788678727786 30.8655240015933110   T   T   T
  0.1029000615869349  0.0406318163968267 30.8568619017161971   T   T   T
  4.4245499049603927 -0.0254166937619170 24.7333408388092550   T   T   T
  0.8209433727949020  3.7001006512548376 26.8377341465829709   T   T   T
  1.5235501999318328  2.4872292184694289 28.8420853590138613   T   T   T
  0.1404973057956387  2.5051425680020363 24.8067431080624132   T   T   T
  0.1021437226774247  2.4958390500954910 30.8586584940634090   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Ni E_tot= -207.13084065 eV
 D3-zero damping= -3.012866 eV, D3-BJ damping= -4.397154 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.2502068721891453    0.0000000000000000    0.0000000000000000
    -2.1251034360945713    3.6807871226550009    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.9233740443146594
   2   5   3   6   3   7   4
Selective dynamics
Cartesian
  2.1917060228742518  0.1572168107471371  9.0169746245084816   F   F   F
 -1.0671842888935670  2.0303823814487334 10.8612336967246357   F   F   F
  1.9660478532346397  2.2436782542207063 11.6081185941916658   F   F   F
  2.9829968896453125  1.2088184299614579  9.5654178022134708   F   F   F
 -0.5370233040116711  3.2200709804448540 10.2987723773365900   F   F   F
  0.9457370778976072  2.9406022105102636  8.2518078419286880   F   F   F
 -0.1670197481133200  1.4709572709156320 11.9218080039603862   F   F   F
  2.2328326002957710 -0.0383913505772471 14.5050718430130097   F   F   F
  1.0458649988794058  1.7218076454770554 12.6701466762358947   F   F   F
 -1.2872892318380489  2.0063957036238902 16.4691297792756650   T   T   T
  1.4491653149646464  2.2195752767649419 17.0072799666788406   T   T   T
  3.2188562276222830  1.0805698283045087 15.1612859962597479   T   T   T
  1.4871512310294490  0.5146828722841187 13.2917821082657603   F   F   F
 -0.8286952737436967  3.4112249019728083 15.8251521933013120   T   T   T
  0.9054819163483715  2.6333005276083892 13.8903255655927040   F   F   F
 -0.6793138384816525  1.4777730706249381 17.8855203754356999   T   T   T
 -0.2920087374567640  3.2261659139736669 20.3961638976988446   T   T   T
  0.8408524186855162  1.6916978656183985 18.4285074417321191   T   T   T
  2.6843527673532188  1.5080130464488999 22.3639439821483741   T   T   T
  1.7927024477775206  0.2160566014514589 21.8930136085050933   T   T   T
  1.1576141651909979  0.2901076795721597 19.1391114347815723   T   T   T
 -0.9930040099391599  1.8279207191316953 20.8672923258456038   T   T   T
  1.0698314011578207  2.7415298861530335 19.6629395780915992   T   T   T
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 -0.4292221130205662  1.2280407243052884 23.5110283705021281   T   T   T
  1.6649737730340262  2.5092202928918637 23.1204010794949859   T   T   T
  1.1796923952886564  0.5826273945846626  8.0000000000000000   F   F   F
  1.0076504386155114  1.4149055525487657  8.0158744918591065   F   F   F
  1.6902022975707689  3.2876161253059846  8.0308754104330884   F   F   F
  0.7748625894864137  2.0444753924844785 23.3688493655718403   T   T   T
 -0.2467261490088948  0.2178197898759302 23.5143131017024736   T   T   T

Oxidized reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Ni E_tot= -194.60570417
eV
 D3-zero damping= -2.8503088 eV, D3-BJ damping= -4.1863927 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.2502068721891453    0.0000000000000000    0.0000000000000000
    -2.1251034360945713    3.6807871226550009    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.4186522310609178
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.1917060228742518  0.1572168107471371  9.0169746245084816   F   F   F
 -1.0671842888935670  2.0303823814487334 10.8612336967246357   F   F   F
  1.9660478532346397  2.2436782542207063 11.6081185941916658   F   F   F
  2.9829968896453125  1.2088184299614579  9.5654178022134708   F   F   F
 -0.5370233040116711  3.2200709804448540 10.2987723773365900   F   F   F
  0.9457370778976072  2.9406022105102636  8.2518078419286880   F   F   F
 -0.1670197481133200  1.4709572709156320 11.9218080039603862   F   F   F
  2.2328326002957710 -0.0383913505772471 14.5050718430130097   F   F   F
  1.0458649988794058  1.7218076454770554 12.6701466762358947   F   F   F
 -1.1445054590719332  1.9530124284304493 16.5287933313162867   T   T   T
  1.8945650474914268  2.3529227624399973 17.5044157415285326   T   T   T
  3.1682259405659861  1.1493707039135870 15.1161678597959614   T   T   T
  1.4871512310294490  0.5146828722841187 13.2917821082657603   F   F   F
 -0.7002219093879583  3.3851593512896563 15.9009569232440811   T   T   T
  0.9054819163483715  2.6333005276083892 13.8903255655927040   F   F   F
 -0.2251074459999272  1.2117347412136075 17.6281947932391745   T   T   T
 -0.3768366636710613  3.8099367559166959 20.5915199266752253   T   T   T
  0.7628703553989298  2.0297690180973369 18.5908407873366173   T   T   T
  3.3552561061460748  1.7024311503560756 22.4738663325628067   T   T   T
  2.7801960885145398  0.3534255199178078 21.8193967513686928   T   T   T
  0.8452103839034975  1.3822537912223580 20.0984010058295688   T   T   T
 -1.3471188537062020  2.7341707761845102 21.2985955600810222   T   T   T
  0.2027942579267788  3.4692207802455668 19.1066481691771592   T   T   T
  0.5984240650011289  1.5416643652531354 23.1607319038273261   T   T   T
  3.5807207828224099  2.0608723326002925 24.0513547182709608   T   T   T
  1.1796923952886564  0.5826273945846626  8.0000000000000000   F   F   F
  1.0076504386155114  1.4149055525487657  8.0158744918591065   F   F   F
  1.6902022975707689  3.2876161253059846  8.0308754104330884   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Ni E_tot= -65.21703902 eV
 D3-zero damping= -3.420018 eV, D3-BJ damping= -4.2254943 eV
Ni
 1.0000000000000000
     4.2502068721891444    0.0000000000000000    0.0000000000000000
     2.1251034360945722    3.6807871226549991    0.0000000000000000
     0.0000000000000000    0.0000000000000000   21.9758133853619810
  12
Cartesian
  4.9585061929312291  1.2270017851453026  9.9895998775674695
  4.9585061771093297  3.6808598584578669  9.9895998323622592
  4.2502059509158636  2.4538638921055140 13.9944372090852251
  2.1251717187803290  1.2268560216223283  7.9811999905978519
  2.8334027408703193  2.4539307580759346  9.9895998825781707
  1.4167980955638388  2.4537872830549721 11.9861271711918747
```

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  2.1251024736007613  1.2269348309401560 13.9944371989874536
  4.2502751608257947 -0.0000730266200595  7.9812000981523132
  2.1251025104935892  3.6807929337745535 13.9944373017538730
  3.5419015386852264  1.2268581946858119 11.9861272515067103
  4.2502751548749025  2.4537850453326344  7.9811999479367666
  3.5419015147887558  3.6807163213213938 11.9861272036044095

Interface: O-a-SiO2(0001)/fcc(111)_sqrt3/Ir E_tot= -318.83742722 eV
 D3-zero damping= -9.3956378 eV, D3-BJ damping= -10.8710435 eV
Si  O Si  O Si  O  H Ir
 1.0000000000000000
     4.7026274333618803    0.0000000000000000    0.0000000000000000
    -2.3513137166809388    4.0725948218250014    0.0000000000000000
     0.0000000000000024    0.0000000000000042   39.4288434860765307
   2   5   3   6   3   7   2  12
Selective dynamics
Cartesian
  2.4250059300582301  0.1739520238515692  9.0169746245084834   F   F   F
 -1.1807825511370400  2.2465099168919989 10.8612336967246375   F   F   F
  2.1753271894648605  2.4825104347217835 11.6081185941916676   F   F   F
  3.3005271104965943  1.3374931813053657  9.5654178022134726   F   F   F
 -0.5941876707989885  3.5628369595602507 10.2987723773365918   F   F   F
  1.0464076834401357  3.2536196570186022  8.2518078419286898   F   F   F
 -0.1847984517013261  1.6275358408490976 11.9218080039603880   F   F   F
  2.4705102965605361 -0.0424779837446797 14.5050718430130114   F   F   F
  1.1571938927269252  1.9050884138310453 12.6701466762358965   F   F   F
 -1.3657630237367084  2.1675357218732323 16.3682454352630984   T   T   T
  1.8287084874419062  2.3400798565613230 16.9312336705515172   T   T   T
  3.4471690755613720  1.0773532838693261 15.1694635829081488   T   T   T
  1.6454535948258069  0.5694691734941677 13.2917821082657621   F   F   F
 -0.8700240225454410  3.5624969549390735 15.7101908044391294   T   T   T
  1.0018674921674353  2.9136067193452204 13.8903255655927058   F   F   F
 -0.5263847019112974  1.7318502358220798 17.6838607674494277   T   T   T
 -0.2441219823296484  3.7455986238869876 20.1200717571935748   T   T   T
  0.9760724377175120  1.9457171487124707 18.2566833706126346   T   T   T
  3.1722522622955780  1.7898808592592519 21.9728141156583057   T   T   T
  2.4223617260379249  0.4149014686577193 21.5318180805147854   T   T   T
  1.3624950301250531  0.5755151937035894 19.0105274213904210   T   T   T
 -1.1669989370893863  2.4809069857482857 20.5533122779135695   T   T   T
  1.0635833875833005  3.1458117214739034 19.3609051114795001   T   T   T
 -0.1872365468078864  1.4475069499459439 22.8486958650768912   T   T   T
  2.1932535661546524  2.7605160534297064 22.8550158999629538   T   T   T
  1.3052667759099936  0.6446461670207518  8.0000000000000018   F   F   F
  1.1149115180437632  1.5655176011714296  8.0158744918591101   F   F   F
  1.8701187804521184  3.6375720632308046  8.0308754104330919   F   F   F
 -1.7808247580023289  4.0892324874225583 27.0100904854885151   T   T   T
 -0.9818771474333675  2.7327985195198932 29.2390792090533580   T   T   T
  2.1530784597343113  2.7471391494499384 24.8147641538442691   T   T   T
  0.5919237675951191  2.7185522855950937 27.0108939630388427   T   T   T
  1.3726398661559422  1.3817412283450698 29.2309235834265557   T   T   T
  2.1551174926531411  2.7405587210268569 31.4201437579288374   T   T   T
 -0.1905802718995677  1.3799083130429850 31.4197234672561052   T   T   T
  4.5180516559510151  1.3830683454808530 24.8107320778113625   T   T   T
  0.5931239953344964  5.4594811371753611 27.0226583588778055   T   T   T
  1.3734731266712339  4.0957790578578397 29.2305257433220440   T   T   T
 -0.1946475086658274  4.0945442391645246 24.8888344906592778   T   T   T
 -0.1980970771728878  4.0894515922173484 31.4278065673130200   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Ir E_tot= -219.67369024 eV
 D3-zero damping= -2.520458 eV, D3-BJ damping= -3.5896651 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.7026274333618803    0.0000000000000000    0.0000000000000000
```

```
    -2.3513137166809388    4.0725948218250014    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.0437180464376183
   2   5   3   6   3   7   4
Selective dynamics
Cartesian
  2.4250059300582296  0.1739520238515692  9.0169746245084816   F   F   F
 -1.1807825511370402  2.2465099168919993 10.8612336967246357   F   F   F
  2.1753271894648605  2.4825104347217835 11.6081185941916658   F   F   F
  3.3005271104965943  1.3374931813053659  9.5654178022134708   F   F   F
 -0.5941876707989885  3.5628369595602507 10.2987723773365900   F   F   F
  1.0464076834401357  3.2536196570186022  8.2518078419286880   F   F   F
 -0.1847984517013261  1.6275358408490976 11.9218080039603862   F   F   F
  2.4705102965605366 -0.0424779837446797 14.5050718430130097   F   F   F
  1.1571938927269252  1.9050884138310455 12.6701466762358947   F   F   F
 -1.3697486676275337  2.1707377394188154 16.3696664371011096   T   T   T
  1.8207960871052542  2.3398656238863320 16.9248277144331460   T   T   T
  3.4474138612571501  1.0726767148819405 15.1788735349547590   T   T   T
  1.6454535948258071  0.5694691734941678 13.2917821082657603   F   F   F
 -0.8747195329791704  3.5631647857726052 15.7071615339258930   T   T   T
  1.0018674921674353  2.9136067193452204 13.8903255655927040   F   F   F
 -0.5343601070404747  1.7525071732943724 17.6951733297956473   T   T   T
 -0.2211707399719362  3.7918936360800970 20.1349970957727322   T   T   T
  0.9704924183028079  1.9755204953324030 18.2598968430996216   T   T   T
  3.2314555709392407  1.8075171909693377 22.0290772272732305   T   T   T
  2.4935540979682056  0.4365307912841973 21.5500015462652321   T   T   T
  1.3547940558714358  0.6283033153546153 19.0544500082829380   T   T   T
 -1.1407029294940263  2.5491742659321388 20.6207696426642038   T   T   T
  1.0646326975755422  3.1987680339426694 19.3358418920343489   T   T   T
 -0.1186665334620169  1.4185925833179496 22.8764081931703878   T   T   T
  2.2529150324589202  2.7258904282944432 22.9711281114057968   T   T   T
  1.3052667759099936  0.6446461670207519  8.0000000000000000   F   F   F
  1.1149115180437634  1.5655176011714298  8.0158744918591065   F   F   F
  1.8701187804521187  3.6375720632308046  8.0308754104330884   F   F   F
  1.3272827112592582  2.3556326031656125 23.0436855035804804   T   T   T
 -0.0090551323340680  0.4344636216499166 23.0025339421113664   T   T   T

Oxidized reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Ir E_tot= -206.99584711
eV
 D3-zero damping= -2.3873062 eV, D3-BJ damping= -3.4344311 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.7026274333618803    0.0000000000000000    0.0000000000000000
    -2.3513137166809388    4.0725948218250014    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.4186522310609178
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.4250059300582296  0.1739520238515692  9.0169746245084816   F   F   F
 -1.1807825511370402  2.2465099168919993 10.8612336967246357   F   F   F
  2.1753271894648605  2.4825104347217835 11.6081185941916658   F   F   F
  3.3005271104965943  1.3374931813053659  9.5654178022134708   F   F   F
 -0.5941876707989885  3.5628369595602507 10.2987723773365900   F   F   F
  1.0464076834401357  3.2536196570186022  8.2518078419286880   F   F   F
 -0.1847984517013261  1.6275358408490976 11.9218080039603862   F   F   F
  2.4705102965605366 -0.0424779837446797 14.5050718430130097   F   F   F
  1.1571938927269252  1.9050884138310455 12.6701466762358947   F   F   F
 -1.2952046118395868  2.1463747164561253 16.3956855870508065   T   T   T
  1.9824535589784502  2.3948391932381172 17.1032394233551628   T   T   T
  3.4265608676564479  1.0955603684185977 15.1647336601167648   T   T   T
  1.6454535948258071  0.5694691734941678 13.2917821082657603   F   F   F
 -0.8263488364337543  3.5536635680620621 15.7394482721749203   T   T   T
  1.0018674921674353  2.9136067193452204 13.8903255655927040   F   F   F
 -0.3629010028397114  1.6283056595808338 17.6126443338424714   T   T   T
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 -0.1379534635618397  4.2301168395601296 20.2513633862541056   T   T   T
  0.9494657405776983  2.2329011982792553 18.3291315072281691   T   T   T
  3.9303821818428712  1.9408962292771026 22.0035972674209432   T   T   T
  3.1809420166402491  0.6287687589537995 21.4620523976007540   T   T   T
  1.2793385445922747  1.3198552512784059 19.6307863917535528   T   T   T
 -1.0991358544081504  3.0825664574148335 20.8917076554591503   T   T   T
  0.7010940715019945  3.6954999089847145 18.9737313523184099   T   T   T
  0.7356811388652537  1.7946838397790901 22.6424200006119030   T   T   T
  4.1820647631796204  2.2631544812218403 23.5856223706709116   T   T   T
  1.3052667759099936  0.6446461670207519  8.0000000000000000   F   F   F
  1.1149115180437634  1.5655176011714298  8.0158744918591065   F   F   F
  1.8701187804521187  3.6375720632308046  8.0308754104330884   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Ir E_tot= -106.94013146 eV
 D3-zero damping= -6.1232614 eV, D3-BJ damping= -6.5235959 eV
Ir
 1.0000000000000000
     4.7026274333618803    0.0000000000000000    0.0000000000000000
     2.3513137166809401    4.0725948218249997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.5811649222271171
  12
Cartesian
  5.4864084891462452  1.3575215306337221 10.1973726642282934
  5.4864084540848266  4.0725847462958393 10.1973726356270795
  4.7026635878283853  2.7150232475461178 14.5811649222271171
  2.3513120976592536  1.3575339961453150  8.0000000423709920
  3.1350947454278209  2.7150531231366286 10.1973726499082780
  1.5675654285001861  2.7150382812561955 12.3838000721759229
  2.3513498709292273  1.3574916069474934 14.5811649118501006
  4.7026258509002323  0.0000024137672120  8.0000000000000000
  2.3513498860676845  4.0725548650549008 14.5811648828473093
  3.9188791450128124  1.3575066558559188 12.3838000305401774
  4.7026258788566748  2.7150656023433632  8.0000000435518448
  3.9188791822807461  4.0725698781837902 12.3838000612110672

Interface: O-a-SiO2(0001)/fcc(111)_sqrt3/Rh E_tot= -298.2917173 eV
 D3-zero damping= -8.2774786 eV, D3-BJ damping= -10.3081055 eV
Si  O Si  O Si  O  H Rh
 1.0000000000000000
     4.6378478337567808    0.0000000000000000    0.0000000000000000
    -2.3189239168783891    4.0164940429200016    0.0000000000000000
     0.0000000000000024    0.0000000000000042   39.2313945901699270
   2   5   3   6   3   7   2  12
Selective dynamics
Cartesian
  2.3916010058078601  0.1715558011834372  9.0169746245084834   F   F   F
 -1.1645170438292110  2.2155638096386951 10.8612336967246375   F   F   F
  2.1453616380065599  2.4483133748322672 11.6081185941916676   F   F   F
  3.2550617131770161  1.3190689548516934  9.5654178022134726   F   F   F
 -0.5860026210687936  3.5137581934940298 10.2987723773365918   F   F   F
  1.0319932158435623  3.2088004189148793  8.2518078419286898   F   F   F
 -0.1822528173982710  1.6051162208372738 11.9218080039603880   F   F   F
  2.4364785408879301 -0.0418928413284443 14.5050718430130114   F   F   F
  1.1412533237368094  1.8788454536116641 12.6701466762358965   F   F   F
 -1.3779956523677179  2.1540814465385090 16.3776963631309016   T   T   T
  1.7418031988335647  2.3249388781586044 16.9166728043724675   T   T   T
  3.4123959307673211  1.0751592790810227 15.1748577922219123   T   T   T
  1.6227871542982433  0.5616246258303044 13.2917821082657621   F   F   F
 -0.8768855033249712  3.5448474863237251 15.7207830568128077   T   T   T
  0.9880665742934088  2.8734712250156220 13.8903255655927058   F   F   F
 -0.5832344350284475  1.7226178266808270 17.7228818570647491   T   T   T
 -0.2558043845011155  3.7109522875279173 20.1544532437260706   T   T   T
  0.9296798479451930  1.9310129185837004 18.2691106152310709   T   T   T
```

```
  3.0828238636637897  1.7920752374479900 22.0555585975269217   T   T   T
  2.3832113618432675  0.4129944208429409 21.5693585579741196   T   T   T
  1.3119695350899390  0.5647066294763110 19.0259093696423847   T   T   T
 -1.1860317535364373  2.4730075489610250 20.6336604877296068   T   T   T
  1.0437991120688668  3.1155994032462879 19.3833255350942295   T   T   T
 -0.2369571756284599  1.4983323232544763 22.9928140207444649   T   T   T
  2.0423513225828787  2.6366722237686644 22.9935283662197314   T   T   T
  1.2872864744041943  0.6357660417762325  8.0000000000000018   F   F   F
  1.0995533969173452  1.5439522943688619  8.0158744918591065   F   F   F
  1.8443575336750038  3.5874638067018947  8.0308754104330884   F   F   F
 -1.8139217270481880  2.7576861077291928 26.9094499475379152   T   T   T
 -1.0315151603731583  1.4025240457633361 29.0726974748158256   T   T   T
  2.0815711268360371  1.4285179110495643 24.7872449145828213   T   T   T
  0.4968046169685748  1.3818890234961572 26.9111066909518009   T   T   T
  1.3004407410254928  0.0637882106723621 29.0378035236962830   T   T   T
  2.0732507134755647  1.3933625193865729 31.2320797210414547   T   T   T
 -0.2459226029042785  0.0632836759028843 31.2036273380900653   T   T   T
  4.4608510717260375  0.0650454980809216 24.4813524947688101   T   T   T
  0.5038502661213853  4.0781982671285117 26.8639489786696224   T   T   T
  1.2875596281041759  2.7383332485313572 29.0642944614831293   T   T   T
 -0.2114486330871273  2.7231324900718601 24.7703235655917169   T   T   T
 -0.2435595357041394  2.7552109819996713 31.2328331655671256   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Rh E_tot= -218.7371166 eV
 D3-zero damping= -2.5872175 eV, D3-BJ damping= -3.6915529 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.6378478337567808    0.0000000000000000    0.0000000000000000
    -2.3189239168783891    4.0164940429200007    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.0994429878475103
   2   5   3   6   3   7   4
Selective dynamics
Cartesian
  2.3916010058078601  0.1715558011834372  9.0169746245084816   F   F   F
 -1.1645170438292110  2.2155638096386943 10.8612336967246357   F   F   F
  2.1453616380065599  2.4483133748322667 11.6081185941916658   F   F   F
  3.2550617131770165  1.3190689548516932  9.5654178022134708   F   F   F
 -0.5860026210687936  3.5137581934940290 10.2987723773365900   F   F   F
  1.0319932158435623  3.2088004189148789  8.2518078419286880   F   F   F
 -0.1822528173982710  1.6051162208372733 11.9218080039603862   F   F   F
  2.4364785408879301 -0.0418928413284443 14.5050718430130097   F   F   F
  1.1412533237368092  1.8788454536116634 12.6701466762358947   F   F   F
 -1.3691466419070166  2.1504535123974806 16.3824259103997569   T   T   T
  1.7511896962063487  2.3128910363653321 16.9236707476432500   T   T   T
  3.4167546806966209  1.0699181736097643 15.1801452569568749   T   T   T
  1.6227871542982431  0.5616246258303044 13.2917821082657603   F   F   F
 -0.8752454768846682  3.5422932979119288 15.7216497347482065   T   T   T
  0.9880665742934088  2.8734712250156211 13.8903255655927040   F   F   F
 -0.5721716180939826  1.7356104492735296 17.7325527716825206   T   T   T
 -0.2285271542155422  3.7311725063067995 20.1742701744001742   T   T   T
  0.9384262414641369  1.9510648311929766 18.2838833716640821   T   T   T
  3.1779419232127211  1.7729336963428544 22.0819101269598193   T   T   T
  2.4270585402702496  0.4059464643071412 21.6103267735021483   T   T   T
  1.3090012329336802  0.6064926349713524 19.0858666969542341   T   T   T
 -1.1283544415068525  2.4704472218047164 20.6511148718266000   T   T   T
  1.0630320735233565  3.1653830544184252 19.3663502674354966   T   T   T
 -0.1197379997195249  1.3915231900644607 22.9463808416881818   T   T   T
  2.2072450327416422  2.7022850440594732 23.0188741422034404   T   T   T
  1.2872864744041945  0.6357660417762324  8.0000000000000000   F   F   F
  1.0995533969173452  1.5439522943688617  8.0158744918591065   F   F   F
  1.8443575336750038  3.5874638067018942  8.0308754104330884   F   F   F
  1.2812182411579951  2.3263649283023016 23.0993388021332215   T   T   T
 -0.0061422122940933  0.4031052083787894 23.0641024662002678   T   T   T
```

```
Oxidized reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Rh E_tot= -206.0602858 eV
 D3-zero damping= -2.4513914 eV, D3-BJ damping= -3.5334135 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.6378478337567808    0.0000000000000000    0.0000000000000000
    -2.3189239168783891    4.0164940429200007    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.4186522310609178
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.3916010058078601  0.1715558011834372  9.0169746245084816   F   F   F
 -1.1645170438292110  2.2155638096386943 10.8612336967246357   F   F   F
  2.1453616380065599  2.4483133748322667 11.6081185941916658   F   F   F
  3.2550617131770165  1.3190689548516932  9.5654178022134708   F   F   F
 -0.5860026210687936  3.5137581934940290 10.2987723773365900   F   F   F
  1.0319932158435623  3.2088004189148789  8.2518078419286880   F   F   F
 -0.1822528173982710  1.6051162208372733 11.9218080039603862   F   F   F
  2.4364785408879301 -0.0418928413284443 14.5050718430130097   F   F   F
  1.1412533237368092  1.8788454536116634 12.6701466762358947   F   F   F
 -1.2068953949433388  2.1005178122210988 16.4373418513025555   T   T   T
  2.1349675985427252  2.4390979586036150 17.3273098738698330   T   T   T
  3.3618007997698740  1.1262451664287130 15.1497431977894177   T   T   T
  1.6227871542982431  0.5616246258303044 13.2917821082657603   F   F   F
 -0.7738903538259844  3.5194862533504918 15.7820660021037842   T   T   T
  0.9880665742934088  2.8734712250156211 13.8903255655927040   F   F   F
 -0.1776160319703430  1.4568171707096453 17.5107456800245700   T   T   T
 -0.2079078229701540  4.1924315404762478 20.2924145141715719   T   T   T
  0.9480275276662896  2.2151343217857660 18.3817894906897585   T   T   T
  3.8726466664502674  1.8949967700923034 22.0447815086520045   T   T   T
  3.2042010729889845  0.5747381422252341 21.4178365119481739   T   T   T
  1.2060516996411337  1.4202466631329616 19.7822442542809647   T   T   T
 -1.1540505084983430  3.0753623809585138 20.9948233318584911   T   T   T
  0.4568401978123979  3.6688001330089324 18.9064652074661765   T   T   T
  0.7382090876809388  1.7820576765948262 22.6972189139759912   T   T   T
  4.0897123345655260  2.1345702500226960 23.6476780010118333   T   T   T
  1.2872864744041945  0.6357660417762324  8.0000000000000000   F   F   F
  1.0995533969173452  1.5439522943688617  8.0158744918591065   F   F   F
  1.8443575336750038  3.5874638067018942  8.0308754104330884   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Rh E_tot= -87.43546597 eV
 D3-zero damping= -4.9774707 eV, D3-BJ damping= -5.851527 eV
Rh
 1.0000000000000000
     4.6378478337567808    0.0000000000000000    0.0000000000000000
     2.3189239168783904    4.0164940429199998    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.5017793304367331
  12
Cartesian
  5.4108142057622519  1.3387991243054735 10.1752851028337794
  5.4108141403760817  4.0164618613968379 10.1752850133523438
  4.6379466470880759  2.6776412699707026 14.5014161875795899
  2.3188828011512301  1.3388716553935265  8.0003510262368671
  3.0918902315888106  2.6776304420597286 10.1752850060218236
  1.5459663323519763  2.6776043926790640 12.3263602656353140
  2.3190227133217634  1.3388098764875969 14.5014160636995015
  4.6378067377148673  0.0000402027084479  8.0003509285714287
  2.3190226536666607  4.0164725948344362 14.5014160673406369
  3.8648901913752267  1.3387731495742594 12.3263602581955620
  4.6378067323153296  2.6777029147935729  8.0003509576555665
  3.8648901694200579  4.0164357576330119 12.3263602750460386

Interface: O-a-SiO2(0001)/fcc(111)_sqrt3/Os E_tot= -343.94688635 eV
```

```
 D3-zero damping= -8.1427079 eV, D3-BJ damping= -10.0646083 eV
Si  O Si  O Si  O  H Os
 1.0000000000000000
     4.6911111462397965    0.0000000000000000    0.0000000000000000
    -2.3455555731198969    4.0626214246200014    0.0000000000000000
     0.0000000000000024    0.0000000000000042   39.3454287515757670
   2   5   3   6   3   7   2  12
Selective dynamics
Cartesian
  2.4190673212785541  0.1735260318969589  9.0169746245084816   F   F   F
 -1.1778909270225779  2.2410084278643980 10.8612336967246357   F   F   F
  2.1700000201635823  2.4764310028818288 11.6081185941916658   F   F   F
  3.2924444336532095  1.3342177877688786  9.5654178022134708   F   F   F
 -0.5927325617310707  3.5541119108556942 10.2987723773365900   F   F   F
  1.0438451305906882  3.2456518520654689  8.2518078419286880   F   F   F
 -0.1843458978769659  1.6235501604373921 11.9218080039603862   F   F   F
  2.4644602519171066 -0.0423739592043343 14.5050718430130097   F   F   F
  1.1543600349924121  1.9004230335776604 12.6701466762358947   F   F   F
 -1.3784168062794444  2.1696101060646100 16.3710896277389892   T   T   T
  1.7979995683160026  2.3433970225418199 16.9193330105212318   T   T   T
  3.4392740789573986  1.0718791516899777 15.1815393939169407   T   T   T
  1.6414240355395140  0.5680745976741467 13.2917821082657603   F   F   F
 -0.8792095125105686  3.5590854710363016 15.7066176903956993   T   T   T
  0.9994140140083472  2.9064715737236959 13.8903255655927040   F   F   F
 -0.5531626541580412  1.7468610878329334 17.7026225813833982   T   T   T
 -0.2221550309496547  3.7894306403477711 20.1367331682409372   T   T   T
  0.9571393650199425  1.9606688598614441 18.2561353184056117   T   T   T
  3.1704618911508748  1.8414009121320047 22.0440530972172120   T   T   T
  2.4995156634299658  0.4631970901035429 21.5251834369506021   T   T   T
  1.3559722722277721  0.6026426795421286 19.0220973826472317   T   T   T
 -1.1700759454922760  2.5797691652051480 20.6490876550791391   T   T   T
  1.0558976015345971  3.1595431407115986 19.3563760977638708   T   T   T
 -0.2115765819926377  1.5215517086307315 22.9963803685895662   T   T   T
  2.1198474393360391  2.6584969009539590 23.0038641613528654   T   T   T
  1.3020703017739272  0.6430674898967905  8.0000000000000000   F   F   F
  1.1121812058216165  1.5616837975275639  8.0158744918591083   F   F   F
  1.8655390375034639  3.6286639953685182  8.0308754104330902   F   F   F
 -1.7063702601051627  2.7702674576358484 26.9270378960816323   T   T   T
 -0.9154118603378664  1.4139988649797575 29.1994285395928621   T   T   T
  2.1706268787882474  1.4448476155544345 24.8595463629446094   T   T   T
  0.6330413654454078  1.4084414733664741 26.9258471890018392   T   T   T
  1.4201854154286606  0.0515609979429495 29.1729273475255440   T   T   T
  2.1847463945878034  1.4130131582124541 31.3029576702989232   T   T   T
 -0.1483184244403013  0.0532220446665087 31.3286305478025433   T   T   T
  4.5541244970218075  0.0532683626839929 24.5662106291429403   T   T   T
  0.6079144708940702  4.1182179219565525 26.8888764593852692   T   T   T
  1.4301316140232299  2.7524466104469094 29.1980035078384432   T   T   T
 -0.1597348194772239  2.7215097627761469 24.8472361172475438   T   T   T
 -0.1623103209844349  2.7584942319979899 31.3023447089019768   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Os E_tot= -219.5216797 eV
 D3-zero damping= -2.5323497 eV, D3-BJ damping= -3.6076123 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.6911111462397965    0.0000000000000000    0.0000000000000000
    -2.3455555731198969    4.0626214246200014    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.0538125475206996
   2   5   3   6   3   7   4
Selective dynamics
Cartesian
  2.4190673212785541  0.1735260318969589  9.0169746245084816   F   F   F
 -1.1778909270225779  2.2410084278643980 10.8612336967246357   F   F   F
  2.1700000201635823  2.4764310028818288 11.6081185941916658   F   F   F
```

```
  3.2924444336532095  1.3342177877688786  9.5654178022134708   F   F   F
 -0.5927325617310707  3.5541119108556942 10.2987723773365900   F   F   F
  1.0438451305906882  3.2456518520654689  8.2518078419286880   F   F   F
 -0.1843458978769659  1.6235501604373921 11.9218080039603862   F   F   F
  2.4644602519171066 -0.0423739592043343 14.5050718430130097   F   F   F
  1.1543600349924121  1.9004230335776604 12.6701466762358947   F   F   F
 -1.3686384313379032  2.1661192394329638 16.3720157887802777   T   T   T
  1.8094922455911637  2.3341573019596562 16.9248317129165926   T   T   T
  3.4425530242368008  1.0719507796036183 15.1784935815635382   T   T   T
  1.6414240355395140  0.5680745976741467 13.2917821082657603   F   F   F
 -0.8738178865428901  3.5588467922796387 15.7103891178278854   T   T   T
  0.9994140140083472  2.9064715737236959 13.8903255655927040   F   F   F
 -0.5399112264349165  1.7473481935267619 17.7015332004711148   T   T   T
 -0.2224544411644926  3.7785209467571779 20.1418355083937257   T   T   T
  0.9658001655765902  1.9692063641003121 18.2641235090850103   T   T   T
  3.2225454268184772  1.7986606320301846 22.0379861347391071   T   T   T
  2.4816514147993223  0.4286339197955777 21.5605882207286719   T   T   T
  1.3476545040654950  0.6220876618638478 19.0594407357753006   T   T   T
 -1.1388129059437853  2.5327517175423719 20.6254328942752458   T   T   T
  1.0649614931930931  3.1903317087988490 19.3419465116459115   T   T   T
 -0.1179654546180442  1.4107967157464998 22.8877233116471501   T   T   T
  2.2459024675432313  2.7193633394822512 22.9793233067591238   T   T   T
  1.3020703017739272  0.6430674898967905  8.0000000000000000   F   F   F
  1.1121812058216165  1.5616837975275639  8.0158744918591065   F   F   F
  1.8655390375034639  3.6286639953685182  8.0308754104330884   F   F   F
  1.3203822393098741  2.3479341624933987 23.0537502903778417   T   T   T
 -0.0077632277214805  0.4258969292901421 23.0124672775410630   T   T   T

Oxidized reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Os E_tot= -206.84187448
eV
 D3-zero damping= -2.3987515 eV, D3-BJ damping= -3.4516482 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.6911111462397965    0.0000000000000000    0.0000000000000000
    -2.3455555731198969    4.0626214246200014    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.4186522310609178
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.4190673212785541  0.1735260318969589  9.0169746245084816   F   F   F
 -1.1778909270225779  2.2410084278643980 10.8612336967246357   F   F   F
  2.1700000201635823  2.4764310028818288 11.6081185941916658   F   F   F
  3.2924444336532095  1.3342177877688786  9.5654178022134708   F   F   F
 -0.5927325617310707  3.5541119108556942 10.2987723773365900   F   F   F
  1.0438451305906882  3.2456518520654689  8.2518078419286880   F   F   F
 -0.1843458978769659  1.6235501604373921 11.9218080039603862   F   F   F
  2.4644602519171066 -0.0423739592043343 14.5050718430130097   F   F   F
  1.1543600349924121  1.9004230335776604 12.6701466762358947   F   F   F
 -1.2922698037281508  2.1419755609884144 16.3981357537246595   T   T   T
  1.9750208379281575  2.3924989208947602 17.1065130596557680   T   T   T
  3.4214072482255262  1.0957910741184780 15.1636048660747829   T   T   T
  1.6414240355395140  0.5680745976741467 13.2917821082657603   F   F   F
 -0.8246670767703581  3.5499817680438901 15.7430194953199596   T   T   T
  0.9994140140083472  2.9064715737236959 13.8903255655927040   F   F   F
 -0.3642611173202381  1.6213625751029626 17.6170722567301254   T   T   T
 -0.1393456932124046  4.2220352555130516 20.2595707973924810   T   T   T
  0.9452156058603275  2.2299232939755127 18.3346990731680499   T   T   T
  3.9221434270951372  1.9363837312382561 22.0128396144722984   T   T   T
  3.1763871609489129  0.6223199281216938 21.4712302486925601   T   T   T
  1.2729673732275366  1.3237145251569924 19.6419169600058687   T   T   T
 -1.1008322500961643  3.0749468267502511 20.8994109016136989   T   T   T
  0.6947309841251501  3.6927774224893621 18.9768206751008606   T   T   T
  0.7390974580394700  1.7912408974996259 22.6518875797904826   T   T   T
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  4.1739605500683012  2.2607100802709867 23.5942814766395514   T   T   T
  1.3020703017739272  0.6430674898967905  8.0000000000000000   F   F   F
  1.1121812058216165  1.5616837975275639  8.0158744918591065   F   F   F
  1.8655390375034639  3.6286639953685182  8.0308754104330884   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Os E_tot= -131.66202437 eV
 D3-zero damping= -4.9347895 eV, D3-BJ damping= -5.6826056 eV
Os
 1.0000000000000000
     4.6911111462397965    0.0000000000000000    0.0000000000000000
     2.3455555731198983    4.0626214246199996    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.5181175745043944
  12
Cartesian
  5.4729713275382945  1.3542633401464219 10.1234824116889346
  5.4729712915703885  4.0626775841355238 10.1234824332284923
  4.6911718731439196  2.7084053483967452 14.5181175240911422
  2.3455395212486621  1.3541817919957424  8.0000000644248210
  3.1274157730324705  2.7084705052898488 10.1234824187008581
  1.5637178571295671  2.7083198732010878 12.3946422896051978
  2.3456162758842845  1.3541982087791373 14.5181175745043980
  4.6910950931724695 -0.0000253472406302  8.0000000000000000
  2.3456163511148400  4.0626124902989318 14.5181174973710174
  3.9092735477788745  1.3541127452899817 12.3946423073664356
  4.6910950253257564  2.7083889149862732  8.0000001299296297
  3.9092735372334895  4.0625270047634157 12.3946422904132660

Interface: O-a-SiO2(0001)/fcc(111)_sqrt3/Ru E_tot= -320.27820014 eV
 D3-zero damping= -8.0433377 eV, D3-BJ damping= -10.0897712 eV
Si  O Si  O Si  O  H Ru
 1.0000000000000000
     4.6179847559130716    0.0000000000000000    0.0000000000000000
    -2.3089923779565344    3.9992921129100010    0.0000000000000000
     0.0000000000000024    0.0000000000000042   39.2287574632877210
   2   5   3   6   3   7   2  12
Selective dynamics
Cartesian
  2.3813582038332695  0.1708210581828920  9.0169746245084834   F   F   F
 -1.1595296243361550  2.2060749436827560 10.8612336967246375   F   F   F
  2.1361734354725161  2.4378276838623902 11.6081185941916676   F   F   F
  3.2411208624823655  1.3134196169970238  9.5654178022134726   F   F   F
 -0.5834928760111430  3.4987093917603151 10.2987723773365918   F   F   F
  1.0275733723482063  3.1950576971201015  8.2518078419286898   F   F   F
 -0.1814722609787895  1.5982417933904238 11.9218080039603880   F   F   F
  2.4260435364080650 -0.0417134217359461 14.5050718430130114   F   F   F
  1.1363655386215279  1.8707986925192117 12.6701466762358965   F   F   F
 -1.3733168817488366  2.1465504203710877 16.3787400627417661   T   T   T
  1.7220008906117674  2.3102532240268525 16.9050365971396523   T   T   T
  3.4078643116773857  1.0720813330797372 15.1738606164840579   T   T   T
  1.6158370453845818  0.5592192873928045 13.2917821082657621   F   F   F
 -0.8761993478517308  3.5390962614591355 15.7245834562165889   T   T   T
  0.9838348607953703  2.8611646585498760 13.8903255655927058   F   F   F
 -0.5912032639083838  1.7246983323350502 17.7350275128812775   T   T   T
 -0.2312824071804324  3.7122469697887248 20.1641947459223339   T   T   T
  0.9260046747142330  1.9329454975163822 18.2717367072976131   T   T   T
  3.1129708478511997  1.7903582395690403 22.0779137035178543   T   T   T
  2.4080375944539600  0.4172796491080212 21.5836877722038629   T   T   T
  1.3059416536553352  0.5768650092603873 19.0457569352889244   T   T   T
 -1.1490566572396392  2.4684227096089022 20.6518777579901354   T   T   T
  1.0606268705031348  3.1272603978153009 19.3725509350811613   T   T   T
 -0.2001707545527603  1.4855782466288183 23.0310972614744074   T   T   T
  2.0917411413691722  2.6312208511680706 23.0411199446931860   T   T   T
  1.2817732552635972  0.6330431688336852  8.0000000000000018   F   F   F
```

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  1.0948442051760128  1.5373398211465181  8.0158744918591101   F   F   F
  1.8364584782130347  3.5720993369287912  8.0308754104330919   F   F   F
 -1.6212050476575521  2.7203252893168886 26.9014345434703763   T   T   T
 -0.8633594229334445  1.4058581585910004 29.1351741371937862   T   T   T
  2.1660796432925511  1.4467325704150304 24.8642956586067463   T   T   T
  0.6781377918547119  1.4026044410804814 26.8997769884015163   T   T   T
  1.4306488978773733  0.0596329830018380 29.1052556819935404   T   T   T
  2.1975289804836793  1.4070123183879226 31.2029880201786334   T   T   T
 -0.1004042050817232  0.0629397883013929 31.2272218649195601   T   T   T
  4.5085196618143737  0.0616023499177987 24.5492075207678013   T   T   T
  0.6412392121648861  4.0593584435735446 26.8473340114483676   T   T   T
  1.4463155597972033  2.7188037466114348 29.1358370967012590   T   T   T
 -0.1249582153738971  2.6738063035113924 24.8444474922402065   T   T   T
 -0.1130468058052129  2.7214098621178398 31.2023532999907900   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Ru E_tot= -218.40536379 eV
 D3-zero damping= -2.6069547 eV, D3-BJ damping= -3.7221747 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.6179847559130716    0.0000000000000000    0.0000000000000000
    -2.3089923779565349    3.9992921129100010    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.1210297204127997
   2   5   3   6   3   7   4
Selective dynamics
Cartesian
  2.3813582038332695  0.1708210581828920  9.0169746245084816   F   F   F
 -1.1595296243361553  2.2060749436827560 10.8612336967246357   F   F   F
  2.1361734354725161  2.4378276838623902 11.6081185941916658   F   F   F
  3.2411208624823655  1.3134196169970238  9.5654178022134708   F   F   F
 -0.5834928760111433  3.4987093917603151 10.2987723773365900   F   F   F
  1.0275733723482059  3.1950576971201015  8.2518078419286880   F   F   F
 -0.1814722609787896  1.5982417933904236 11.9218080039603862   F   F   F
  2.4260435364080650 -0.0417134217359461 14.5050718430130097   F   F   F
  1.1363655386215277  1.8707986925192117 12.6701466762358947   F   F   F
 -1.3660641002813458  2.1436554062455566 16.3885677620365975   T   T   T
  1.7337423129849747  2.3040400219755370 16.9288054675977548   T   T   T
  3.4069173344830985  1.0692517679439937 15.1817139128771377   T   T   T
  1.6158370453845818  0.5592192873928045 13.2917821082657603   F   F   F
 -0.8748595027597080  3.5350891380492704 15.7261850611072749   T   T   T
  0.9838348607953700  2.8611646585498756 13.8903255655927040   F   F   F
 -0.5795230031209534  1.7274852266323657 17.7448347940648397   T   T   T
 -0.2299612890853125  3.7080926784435406 20.1908987465602436   T   T   T
  0.9318331487647672  1.9398297936148778 18.2951745468774156   T   T   T
  3.1604689999343942  1.7589555221487958 22.1031012391983737   T   T   T
  2.4052356745979475  0.3934220978773572 21.6332585609110843   T   T   T
  1.2970434093892274  0.5955548897569450 19.0991687254863152   T   T   T
 -1.1248450205993976  2.4429301909981076 20.6658714590209627   T   T   T
  1.0632986535462039  3.1504925743371497 19.3808823232027514   T   T   T
 -0.1222455235836474  1.3812699409018609 22.9754911674352265   T   T   T
  2.1914575526879534  2.6912208994388580 23.0375993983807348   T   T   T
  1.2817732552635974  0.6330431688336852  8.0000000000000000   F   F   F
  1.0948442051760123  1.5373398211465181  8.0158744918591065   F   F   F
  1.8364584782130342  3.5720993369287912  8.0308754104330884   F   F   F
  1.2648471680314923  2.3143656722047297 23.1199520244708836   T   T   T
 -0.0061359202379870  0.3916411184225397 23.0898487126751100   T   T   T

Oxidized reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Ru E_tot= -205.72230719
eV
 D3-zero damping= -2.4704962 eV, D3-BJ damping= -3.562663 eV
Si  O Si  O Si  O  H
 1.0000000000000000
     4.6179847559130716    0.0000000000000000    0.0000000000000000
    -2.3089923779565349    3.9992921129100010    0.0000000000000000
```

```
     0.0000000000000019    0.0000000000000033   31.4186522310609178
   2   5   3   6   3   7   2
Selective dynamics
Cartesian
  2.3813582038332695  0.1708210581828920  9.0169746245084816   F   F   F
 -1.1595296243361553  2.2060749436827560 10.8612336967246357   F   F   F
  2.1361734354725161  2.4378276838623902 11.6081185941916658   F   F   F
  3.2411208624823655  1.3134196169970238  9.5654178022134708   F   F   F
 -0.5834928760111433  3.4987093917603151 10.2987723773365900   F   F   F
  1.0275733723482059  3.1950576971201015  8.2518078419286880   F   F   F
 -0.1814722609787896  1.5982417933904236 11.9218080039603862   F   F   F
  2.4260435364080650 -0.0417134217359461 14.5050718430130097   F   F   F
  1.1363655386215277  1.8707986925192117 12.6701466762358947   F   F   F
 -1.1975365102077911  2.0918247745337912 16.4444430185829553   T   T   T
  2.1360885308662572  2.4362512734429620 17.3486661769256933   T   T   T
  3.3511304060212548  1.1274561871809607 15.1491783869382299   T   T   T
  1.6158370453845818  0.5592192873928045 13.2917821082657603   F   F   F
 -0.7689397109900847  3.5115613079395782 15.7885121960798092   T   T   T
  0.9838348607953700  2.8611646585498756 13.8903255655927040   F   F   F
 -0.1668819947944559  1.4404463822792404 17.5120657467824898   T   T   T
 -0.2101535479982161  4.1759184935987905 20.3094366329418214   T   T   T
  0.9437567299516840  2.2066905045578586 18.3950477038184204   T   T   T
  3.8585611093042673  1.8846986348387036 22.0682602655615803   T   T   T
  3.1975253538978925  0.5645737187945753 21.4328862715174893   T   T   T
  1.1931995982095494  1.4230225933496214 19.8042989341653914   T   T   T
 -1.1548004378856129  3.0621441181837477 21.0174783335963049   T   T   T
  0.4412814786169734  3.6586869067130960 18.9143352078186737   T   T   T
  0.7430215227912502  1.7753517157033611 22.7235681704431904   T   T   T
  4.0714646612304515  2.1206639297409291 23.6723410586875147   T   T   T
  1.2817732552635974  0.6330431688336852  8.0000000000000000   F   F   F
  1.0948442051760123  1.5373398211465181  8.0158744918591065   F   F   F
  1.8364584782130342  3.5720993369287912  8.0308754104330884   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt3/Ru E_tot= -108.70923104 eV
 D3-zero damping= -4.7429262 eV, D3-BJ damping= -5.6232816 eV
Ru
 1.0000000000000000
     4.6179847559130716    0.0000000000000000    0.0000000000000000
     2.3089923779565358    3.9992921129099992    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.4084815249538565
  12
Cartesian
  5.3877199732719454  1.3330671769786648 10.0948982599007611
  5.3876921316083086  3.9992800040548420 10.0948848681609267
  4.6180363988259918  2.6661662101717183 14.4091451294994801
  2.3089084437188805  1.3330701002028027  7.9992881352323799
  3.0786258182463726  2.6662217864006115 10.0949228697323594
  1.5393391741777305  2.6661811884859241 12.3135791330974556
  2.3090901342500652  1.3330785067888125 14.4091996535252846
  4.6179610423846977 -0.0000268395427653  7.9992451285714274
  2.3090480515514482  3.9992383029447227 14.4091666204827256
  3.8483377229941835  1.3330847420037120 12.3135932515719038
  4.6179538097811115  2.6661963023548161  7.9992814524803357
  3.8483403818493844  3.9992736049538200 12.3135768863677395

Interface: ZrO2(101)/fcc(100)_7x4/Ag E_tot= -2288.86530056 eV
 D3-zero damping= -67.2152701 eV, D3-BJ damping= -83.0477893 eV
 O Zr Ag
 1.0000000000000000
    20.1636893636500041    0.0000000000000000    0.0000000000000000
     0.0000000000000000   11.5221082078000023    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.7350387248916377
 144  72  84
```

Selective dynamics
Cartesian

3.5442444978160266	1.9203515167996819	8.0000000000000000	F	F	F
6.4197561315259595	0.0000000782460909	8.3161459287561925	F	F	F
1.2645512113273771	1.9203516483643084	9.4856979795260195	F	F	F
4.1400629267387519	0.0000002499831350	9.8018440286466415	F	F	F
5.7060908087574314	1.9203517029389625	10.9713994226004097	F	F	F
1.8603726545840267	0.0000002643853721	11.2875453513566022	F	F	F
3.4263975222687817	1.9203518345035895	12.4570974021264291	F	F	F
6.3019092376801558	0.0000004361224159	12.7732434512470512	F	F	F
1.1658536669981883	1.9785299753540999	13.8539162198046988	T	T	T
3.8199481388721148	0.1344755726395526	14.1537650432441389	T	T	T
5.5111855135229852	2.1834981738628798	15.2031775991578986	T	T	T
1.5309988536463337	-0.2630854122781203	15.6432173369935317	T	T	T
3.1417038705971896	1.9076031378282874	16.5717620505165470	T	T	T
5.7357936952014379	0.3734223360447279	17.0479408171078752	T	T	T
0.7547191042956904	1.5044095125441497	17.9471966339821130	T	T	T
3.4135886304111360	-0.3062870662406695	18.3735762327389764	T	T	T
3.5442441804275280	5.7610542527330022	8.0000000000000000	F	F	F
6.4197558141374609	3.8407028141794117	8.3161459287561925	F	F	F
1.2645508939388781	5.7610543842976289	9.4856979795260195	F	F	F
4.1400626093502533	3.8407029859164554	9.8018440286466415	F	F	F
5.7060904913689328	5.7610544388722831	10.9713994226004097	F	F	F
1.8603723371955281	3.8407030003186926	11.2875453513566022	F	F	F
3.4263972048802831	5.7610545704369107	12.4570974021264291	F	F	F
6.3019089202916572	3.8407031720557367	12.7732434512470512	F	F	F
1.1123546818176369	5.7818188105543120	13.8409794998532476	T	T	T
3.9294873588071613	4.0268563126263617	14.1670234948853366	T	T	T
5.7900871824877509	6.1405050128022518	15.3571222192606918	T	T	T
1.6013079363913696	3.7418035829793719	15.5884297273362105	T	T	T
3.3819292402641570	5.8495985669856676	16.5793478558312160	T	T	T
5.6572108460184563	4.0870835676451094	16.9249882480463079	T	T	T
0.8993100538218984	5.4172957655019509	17.9560299433190700	T	T	T
3.4353357785335317	3.4288469971367093	18.5137992138380127	T	T	T
3.5442438630390298	9.6017569886663221	8.0000000000000000	F	F	F
6.4197554967489623	7.6814055501127330	8.3161459287561925	F	F	F
1.2645505765503795	9.6017571202309497	9.4856979795260195	F	F	F
4.1400622919617538	7.6814057218497762	9.8018440286466415	F	F	F
5.7060901739804342	9.6017571748056039	10.9713994226004097	F	F	F
1.8603720198070293	7.6814057362520138	11.2875453513566022	F	F	F
3.4263968874917845	9.6017573063702297	12.4570974021264291	F	F	F
6.3019086029031568	7.6814059079890571	12.7732434512470512	F	F	F
1.1310861801361132	9.6212411836389382	13.8489379121896885	T	T	T
3.8918651832068094	7.8148664599426674	14.1685490239455767	T	T	T
5.5498955364417117	9.9534846189891049	15.2693256727904672	T	T	T
1.5452674839557239	7.4322478560363638	15.6074359376367688	T	T	T
3.1810503930734679	9.4108776271498567	16.6217474823006910	T	T	T
5.8207433478664097	8.1585590226021161	17.0749802393342485	T	T	T
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Oxide reference: ZrO2(101)/fcc(100)_7x4/Ag E_tot= -2044.12648039 eV
 D3-zero damping= -28.126246 eV, D3-BJ damping= -40.8110596 eV
 O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr
O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr
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     0.0000000000000000   11.5221082078000023    0.0000000000000000
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2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2   4
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2   4   2   2   1   2   1   4   2   4   2   4   2   2   1
Selective dynamics
Cartesian
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  1.2645512113273771  1.9203516483643084  9.4856979795260195   F   F   F
  4.1400629267387519  0.0000002499831350  9.8018440286466415   F   F   F
  5.7060908087574314  1.9203517029389625 10.9713994226004097   F   F   F
  1.8603726545840267  0.0000002643853721 11.2875453513566022   F   F   F
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  5.5224613781948504  1.9203515359249641  8.9009233068204310   F   F   F
  3.4263975222687817  1.9203518345035895 12.4570974021264291   F   F   F
  6.3019092376801558  0.0000004361224159 12.7732434512470512   F   F   F
  1.2160099547281134  1.9379493084540791 13.8541045499284792   T   T   T
  4.0210391503603100  0.1905654684381557 14.1702904269092116   T   T   T
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18.9649206365730230	5.7610542718582840	8.9009233068204310	F	F	F
16.8688567806469543	5.7610545704369107	12.4570974021264291	F	F	F
19.7443684960583283	3.8407031720557367	12.7732434512470512	F	F	F
14.7262199157659701	6.1163682672868633	13.8739108171243561	T	T	T
17.3122643718256164	3.6694290440380430	14.1394013196767361	T	T	T
19.9625175197173697	3.4641357105393165	14.8339853416524825	T	T	T
14.4055371596310913	5.7610544579975658	11.8723227294208407	F	F	F
18.9733477195281068	5.4552219671045146	15.1361590486907769	T	T	T

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 15.0067361387855360  3.9850782028479395 15.6611467873481800   T   T   T
 16.7047223263731475  5.8438342346615570 16.5873783527225136   T   T   T
 19.2812337384191714  3.5723353084313993 16.8818043329530632   T   T   T
 15.4360559633113912  4.2207049873724216 17.7162516409037636   T   T   T
 16.5617626497602259  5.5371193615038417 14.5918207019912103   T   T   T
 13.9839895558560965  5.4700699645401345 18.2184428346481369   T   T   T
 17.2367575344929271  4.5210276052859841 18.6472190719242015   T   T   T
 18.5154162651077172  5.3543983728068705 17.3772175468062251   T   T   T
 16.9867034388056943  9.6017569886663221  8.0000000000000000   F   F   F
 19.8622150725156281  7.6814055501127330  8.3161459287561925   F   F   F
 15.6043049849171105  7.6814056632841625  8.9009207394719176   F   F   F
 14.7070101523170482  9.6017571202309497  9.4856979795260195   F   F   F
 17.5825218677284241  7.6814057218497762  9.8018440286466415   F   F   F
 19.1485497497471009  9.6017571748056039 10.9713994226004097   F   F   F
 15.3028315955737000  7.6814057362520138 11.2875453513566022   F   F   F
 17.7661512958585135  7.6814058494234434 11.8723201620723273   F   F   F
 18.9649203191845217  9.6017570077916066  8.9009233068204310   F   F   F
 16.8688564632584530  9.6017573063702297 12.4570974021264291   F   F   F
 19.7443681786698271  7.6814059079890571 12.7732434512470512   F   F   F
 14.5851613932647801  9.5899989141839281 13.8921975770521797   T   T   T
 17.3665827903288630  7.6100956822285228 14.1920141821009800   T   T   T
 19.9490566723919223  7.2391617043994811 14.8195773101194099   T   T   T
 14.4055368422425936  9.6017571939308848 11.8723227294208407   F   F   F
 19.3552979699921224  9.2813607495364039 15.3220002364662093   T   T   T
 15.1091364863559203  8.1988652896301595 15.9084447561298958   T   T   T
 17.1329756295550304  9.8245554249799820 16.5718046686736464   T   T   T
 19.4356313848517921  7.2087982289872885 16.9824791497260748   T   T   T
 15.8906304723566780  8.7641926165867527 17.7464750289564428   T   T   T
 16.5261637440190761  9.4360440632890441 14.5866789253355336   T   T   T
 15.0550571351102818 10.3576372364998388 18.4143125543354493   T   T   T
 17.6260160067648108  8.4287885573540677 18.6710519820999394   T   T   T
 19.0678660540186051  9.1509837767250470 17.4585642381818431   T   T   T

Metal reference: ZrO2(101)/fcc(100)_7x4/Ag E_tot= -229.08748835 eV
 D3-zero damping= -25.1541628 eV, D3-BJ damping= -31.6641461 eV
Ag
 1.0000000000000000
    20.1636893636500041    0.0000000000000000    0.0000000000000000
     0.0000000000000000   11.5221082078000023    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9359299014895974
  84
Cartesian
  0.0000000000000000  0.0000000000000000  7.9087772701206296
  1.4403366850972428  1.4402635259750003  9.9730482836313623
 -0.0000000000000000  0.0000000000000000 12.0376427737215614
 -0.0000000000000000  2.8805270519500006  7.9087772701206296
  1.4403366850972432  4.3207905779250009  9.9730482836313623
  0.0000000000000000  2.8805270519500006 12.0376427737215614
  0.0000000000000000  5.7610541039000012  7.9087772701206296
  1.4403366850972432  7.2013176298750015  9.9730482836313623
  0.0000000000000000  5.7610541039000012 12.0376427737215614
 -0.0000000000000000  8.6415811558500017  7.9087772701206296
  1.4403366850972432 10.0818446818250020  9.9730482836313623
 -0.0000000000000000  8.6415811558500017 12.0376427737215614
  2.8811825508601077  0.0000000000000000  7.9079686201672512
  4.3207453700785869  1.4402635259750003  9.9731423850242731
  2.8805508786897156 -0.0000000000000000 12.0380564501463443
  2.8811825508601077  2.8805270519500006  7.9079686201672512
  4.3207453700785869  4.3207905779250009  9.9731423850242731
  2.8805508786897156  2.8805270519500006 12.0380564501463443
  2.8811825508601077  5.7610541039000012  7.9079686201672512
  4.3207453700785869  7.2013176298750015  9.9731423850242731
  2.8805508786897156  5.7610541039000012 12.0380564501463443
```

2.8811825508601077	8.6415811558500017	7.9079686201672512
4.3207453700785869	10.0818446818250020	9.9731423850242731
2.8805508786897156	8.6415811558500017	12.0380564501463443
5.7616478604007941	-0.0000000000000000	7.9081850946666306
7.2009139327344922	1.4402635259750003	9.9731104505205330
5.7616030363098609	-0.0000000000000000	12.0380648116156141
5.7616478604007941	2.8805270519500006	7.9081850946666306
7.2009139327344922	4.3207905779250009	9.9731104505205330
5.7616030363098609	2.8805270519500006	12.0380648116156141
5.7616478388471579	5.7610541039000012	7.9081850946666306
7.2009139327344922	7.2013176298750015	9.9731104173571836
5.7616030363098609	5.7610541039000012	12.0380647900619770
5.7616478388471579	8.6415811558500017	7.9081850946666306
7.2009139327344922	10.0818446818250020	9.9731104505205330
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8.6418402130317791	-0.0000000000000000	7.9085140072257154
10.0818446818250020	1.4402635259750003	9.9729359944852689
8.6422550787576800	0.0000000000000000	12.0380075008656622
8.6418402130317791	2.8805270519500006	7.9085140072257154
10.0818446818250020	4.3207905779250009	9.9729359944852689
8.6422550787576800	2.8805270519500006	12.0380075008656622
8.6418402130317791	5.7610541039000012	7.9085140072257154
10.0818446818250020	7.2013176298750015	9.9729359944852689
8.6422550787576800	5.7610541039000012	12.0380075008656622
8.6418402130317791	8.6415811558500017	7.9085140072257154
10.0818446818250020	10.0818446818250020	9.9729359944852689
8.6422550787576800	8.6415811558500017	12.0380075008656622
11.5218491506182250	-0.0000000000000000	7.9085140072257154
12.9627754309155225	1.4402635259750003	9.9731104173571836
11.5214342848923241	-0.0000000000000000	12.0380075008656622
11.5218491506182250	2.8805270519500006	7.9085140072257154
12.9627754309155225	4.3207905779250009	9.9731104173571836
11.5214342848923241	2.8805270519500006	12.0380075008656622
11.5218491506182250	5.7610541039000012	7.9085140072257154
12.9627754309155225	7.2013176298750015	9.9731104173571836
11.5214342848923241	5.7610541039000012	12.0380075008656622
11.5218491506182250	8.6415811558500017	7.9085140072257154
12.9627754309155225	10.0818446818250020	9.9731104173571836
11.5214342848923241	8.6415811558500017	12.0380075008656622
14.4020415248028453	0.0000000000000000	7.9081850946666341
15.8429439935714100	1.4402635259750003	9.9731423850242731
14.4020863273401485	-0.0000000000000000	12.0380647900619770
14.4020415248028453	2.8805270519500006	7.9081850946666306
15.8429439935714100	4.3207905779250009	9.9731423850242731
14.4020863273401485	2.8805270519500006	12.0380647900619770
14.4020415248028453	5.7610541039000012	7.9081850578502388
15.8429439935714100	7.2013176298750015	9.9731423850242731
14.4020863273401378	5.7610541039000012	12.0380647900619770
14.4020415248028453	8.6415811558500017	7.9081850946666306
15.8429439935714100	10.0818446818250020	9.9731423850242731
14.4020863273401378	8.6415811558500017	12.0380647900619770
17.2825068127898582	0.0000000000000000	7.9079686201672512
18.7233526785527431	1.4402635259750003	9.9730482836313623
17.2831384849602969	0.0000000000000000	12.0380565113552738
17.2825068127898582	2.8805270519500006	7.9079686201672512
18.7233526785527431	4.3207905779250009	9.9730482836313623
17.2831384849602969	2.8805270519500006	12.0380565113552738
17.2825068127898582	5.7610541039000012	7.9079686201672512
18.7233526785527431	7.2013176298750015	9.9730482836313623
17.2831384849602969	5.7610541039000012	12.0380565113552738
17.2825068127898582	8.6415811558500017	7.9079686201672512
18.7233526785527431	10.0818446818250020	9.9730482836313623
17.2831384849602969	8.6415811558500017	12.0380565113552738

```
Interface: ZrO2(101)/fcc(100)_7x4/Cu E_tot= -2376.36640825 eV
 D3-zero damping= -68.6524004 eV, D3-BJ damping= -90.1653612 eV
 O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr
O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr Cu
 1.0000000000000000
    17.6663874571100052    0.0000000000000000    0.0000000000000000
     0.0000000000000000   10.0950785469200017    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.7141006455589860
   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2   4   2
2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2   4
2   2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2
4   2   2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4
2   4   2   2   1   2   1   4   2   4   2   4   2   2   1  84
Selective dynamics
Cartesian
  3.1052847230440519  1.6825132215531657  8.0000000000000000   F   F   F
  5.6246601082910761  0.0000000685552001  8.3161459287561925   F   F   F
  1.8940983044250344  0.0000001677101859  8.9009207394719176   F   F   F
  1.1079347264167172  1.6825133368233240  9.4856979795260195   F   F   F
  3.6273101832463417  0.0000002190223645  9.8018440286466415   F   F   F
  4.9993832614129898  1.6825133846388289 10.9713994226004097   F   F   F
  1.6299628276233433  0.0000002316408638 11.2875453513566022   F   F   F
  3.7881968427939716  0.0000003307958494 11.8723201620723273   F   F   F
  4.8384965997341363  1.6825132383097543  8.9009233068204310   F   F   F
  3.0020332647856547  1.6825134999089877 12.4570974021264291   F   F   F
  5.5214087216152796  0.0000003821080279 12.7732434512470512   F   F   F
  1.0502555112770220  1.6851703022316431 14.1825164451805730   T   T   T
  3.4913447262575366 -0.0000074604353065 14.5459855648951724   T   T   T
  5.6434752736249072 -0.0000053613975580 14.9007572331056295   T   T   T
  0.8437993190664066  1.6825134013954173 11.8723227294208407   F   F   F
  4.8791070947001467  1.6853113526719892 15.8566954757855303   T   T   T
  1.4499884749408514  0.0000040586091963 16.2563080674149916   T   T   T
  2.8260733270798672  1.6810898710352993 17.6938840299467195   T   T   T
  5.2662781004459340 -0.0000162452423968 18.2291706690610162   T   T   T
  1.5195286195523345  0.0000122787876004 18.3882129828256886   T   T   T
  2.7677512751713178  1.6835826835475600 15.5452701038796448   T   T   T
  0.7417916386420588  1.6954424160300150 19.4298556586687639   T   T   T
  3.1440013265940130  0.0000066322559880 19.7359611362713920   T   T   T
  4.5155474394538331  1.6817738584671356 19.1851133889138481   T   T   T
  3.1052844449645751  5.0475394038598207  8.0000000000000000   F   F   F
  5.6246598302115984  3.3650262508618560  8.3161459287561925   F   F   F
  1.8940980263455574  3.3650263500168411  8.9009207394719176   F   F   F
  1.1079344483372400  5.0475395191299794  9.4856979795260195   F   F   F
  3.6273099051668654  3.3650264013290196  9.8018440286466415   F   F   F
  4.9993829833335122  5.0475395669454839 10.9713994226004097   F   F   F
  1.6299625495438663  3.3650264139475197 11.2875453513566022   F   F   F
  3.7881965647144948  3.3650265131025048 11.8723201620723273   F   F   F
  4.8384963216546595  5.0475394206164097  8.9009233068204310   F   F   F
  3.0020329867061775  5.0475396822156435 12.4570974021264291   F   F   F
  5.5214084435358020  3.3650265644146833 12.7732434512470512   F   F   F
  1.0516692020886602  5.0475419933559031 14.1843989393794594   T   T   T
  3.4911411753123573  3.3676414956229856 14.5465715192309997   T   T   T
  5.6464482677688377  3.3679375903196056 14.9017676423889256   T   T   T
  0.8437990409869295  5.0475395837020738 11.8723227294208407   F   F   F
  4.8752873242569779  5.0475376689456430 15.8602841085400676   T   T   T
  1.4538866242662865  3.3712824065879086 16.2622522172605599   T   T   T
  2.8338080383379571  5.0475446228291840 17.7307048315796010   T   T   T
  5.2687783670756181  3.3882392165601383 18.2561815647449563   T   T   T
  1.5251633933392330  3.3625034657602870 18.3944868902968750   T   T   T
  2.7698996272657146  5.0475384095273101 15.5565661055402611   T   T   T
```

0.7576478172019786	5.0475374721909798	19.4749746567342967	T	T	T
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4.5176656271920095	5.0475318228522736	19.2115923447761503	T	T	T
3.1052841668850983	8.4125655861664761	8.0000000000000000	F	F	F
5.6246595521321225	6.7300524331685114	8.3161459287561925	F	F	F
1.8940977482660803	6.7300525323234979	8.9009207394719176	F	F	F
1.1079341702577630	8.4125657014366357	9.4856979795260195	F	F	F
3.6273096270873877	6.7300525836356755	9.8018440286466415	F	F	F
4.9993827052540354	8.4125657492521402	10.9713994226004097	F	F	F
1.6299622714643893	6.7300525962541755	11.2875453513566022	F	F	F
3.7881962866350181	6.7300526954091611	11.8723201620723273	F	F	F
4.8384960435751836	8.4125656029230651	8.9009233068204310	F	F	F
3.0020327086267011	8.4125658645222980	12.4570974021264291	F	F	F
5.5214081654563234	6.7300527467213387	12.7732434512470512	F	F	F
1.0502541193565422	8.4099094868076207	14.1825246884289928	T	T	T
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5.6464455683154338	6.7271425304960104	14.9017708241885387	T	T	T
0.8437987629074524	8.4125657660087274	11.8723227294208407	F	F	F
4.8791051946516246	8.4097550612230325	15.8567159239140043	T	T	T
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5.2687780658663277	6.7068427302513038	18.2562098330329299	T	T	T
1.5251569948210033	6.7325817503954104	18.3944993424324963	T	T	T
2.7677591333412934	8.4114927114943985	15.5452889708188646	T	T	T
0.7417896495688374	8.3996488011063963	19.4298759616867258	T	T	T
3.1277687476182066	6.7856363696400166	19.7690609458076274	T	T	T
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8.9940805420807202	1.6825132215531657	8.0000000000000000	F	F	F
11.5134559273277475	0.0000000685552001	8.3161459287561925	F	F	F
7.7828941234617037	0.0000001677101859	8.9009207394719176	F	F	F
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7.5187586466600109	0.0000002316408638	11.2875453513566022	F	F	F
9.6769926618306403	0.0000003307958494	11.8723201620723273	F	F	F
10.7272924187708085	1.6825132383097543	8.9009233068204310	F	F	F
8.8908290838223234	1.6825134999089877	12.4570974021264291	F	F	F
11.4102045406519448	0.0000003821080279	12.7732434512470512	F	F	F
6.9212847193216689	1.6863778579437252	14.1902348565456879	T	T	T
9.3565800924991080	-0.0000023444334239	14.5442485998619411	T	T	T
11.5267991553818305	-0.0000096555791340	14.8845627477982436	T	T	T
6.7325951381030746	1.6825134013954173	11.8723227294208407	F	F	F
10.7662948498105262	1.6852770952038958	15.8223940661130165	T	T	T
7.3044019899438464	-0.0000071719506622	16.2779140925040942	T	T	T
8.7472001753084943	1.6796721680290803	17.6547688881027049	T	T	T
11.2065501034946138	-0.0000042328542755	18.0926223336994667	T	T	T
7.4116949543687038	-0.0000043869575901	18.4094833583289272	T	T	T
8.6355725553687197	1.6844441718967220	15.5317800785242053	T	T	T
6.7341836983138199	1.6849020099723084	19.4288128774778244	T	T	T
9.1478609708759961	0.0000083875667583	19.7039160984189543	T	T	T
10.4210983350518891	1.6815207701283308	19.0377107679178081	T	T	T
8.9940802640012443	5.0475394038598207	8.0000000000000000	F	F	F
11.5134556492482663	3.3650262508618560	8.3161459287561925	F	F	F
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Oxide reference: ZrO2(101)/fcc(100)_7x4/Cu E_tot= -2057.80405286 eV
 D3-zero damping= -33.8195619 eV, D3-BJ damping= -48.788249 eV
 O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr
O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
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Selective dynamics
Cartesian
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Metal reference: ZrO2(101)/fcc(100)_7x4/Cu E_tot= -304.58950165 eV
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Interface: ZrO2(101)/fcc(100)_7x4/Pt E_tot= -2590.3534124 eV
 D3-zero damping= -84.4216851 eV, D3-BJ damping= -97.6617597 eV
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Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr
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Cartesian
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Oxide reference: ZrO2(101)/fcc(100)_7x4/Pt E_tot= -2064.61606778 eV
 D3-zero damping= -29.5598815 eV, D3-BJ damping= -43.672341 eV
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Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr
O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
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Metal reference: ZrO2(101)/fcc(100)_7x4/Pt E_tot= -501.9428276 eV
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     0.0000000000000000   11.0818134616800013    0.0000000000000000
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  84
Cartesian
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 18.0075799597509629  4.1554092550960986  9.9395751528688798
 16.6232642419349759  2.7704533654200003 11.8753870245808653
 16.6212061945241594  5.5409067308400006  8.0038400526152760
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 16.6229607445636809  8.3113600962600014  8.0039658246205967
 18.0075800033561961  9.6963159383976052  9.9395751321292138
 16.6232642053533297  8.3113600962600014 11.8753870583576813

Interface: ZrO2(101)/fcc(100)_7x4/Pd E_tot= -2517.29131623 eV
 D3-zero damping= -74.8564806 eV, D3-BJ damping= -92.1526612 eV
 O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr
O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr Pd
 1.0000000000000000
    19.2358686233000036    0.0000000000000000    0.0000000000000000
     0.0000000000000000   10.9919249276000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.5159975464327360
   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2   4   2
2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2   4
2   2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2
4   2   2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4
2   4   2   2   1   2   1   4   2   4   2   4   2   2   1  84
Selective dynamics
Cartesian
  3.3811580955887997  1.8319876299178814  7.9999999999999991   F   F   F
  6.1243546908770714  0.0000000746456413  8.3161459287561925   F   F   F
  2.0623699232222941  0.0000001826095522  8.9009207394719176   F   F   F
  1.2063636038938199  1.8319877554286361  9.4856979795260195   F   F   F
  3.9495602771240876  0.0000002384803027  9.8018440286466451   F   F   F
  5.4435282735385639  1.8319878074920686 10.9713994226004097   F   F   F
  1.7747686610601652  0.0000002522198290 11.2875453513566022   F   F   F
  4.1247401011720575  0.0000003601837396 11.8723201620723273   F   F   F
  5.2683484471700321  1.8319876481631248  8.9009233068204310   F   F   F
  3.2687337818435838  1.8319879330028237 12.4570974021264291   F   F   F
  6.0119304550738519  0.0000004160544901 12.7732434512470512   F   F   F
  1.0899555600255453  1.8453561952777271 13.9315778909806145   T   T   T
  3.8724237391176755  0.0000433859870289 14.2446603343559772   T   T   T
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6.1741712048656279	-0.0001362865166921	14.8608968870602656	T	T	T
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1.6951553152017516	-0.0000449530904527	15.6438164529035824	T	T	T
3.1513301364012882	1.7424389713038693	16.8594107269148559	T	T	T
5.8819233293605775	-0.0002295868090197	17.2149715149793110	T	T	T
1.9083657478872236	-0.0011538563492188	17.7194779092769217	T	T	T
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3.7759950181001649	-0.0004775804283194	18.6956716065106257	T	T	T
5.0505674655668740	1.8656740122167870	17.7812197483864232	T	T	T
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2.0623696204382473	3.6639751584762061	8.9009207394719176	F	F	F
1.2063633011097730	5.4959627312952906	9.4856979795260195	F	F	F
3.9495599743400409	3.6639752143469568	9.8018440286466451	F	F	F
5.4435279707545172	5.4959627833587223	10.9713994226004097	F	F	F
1.7747683582761185	3.6639752280864832	11.2875453513566022	F	F	F
4.1247397983880116	3.6639753360503935	11.8723201620723273	F	F	F
5.2683481443859854	5.4959626240297785	8.9009233068204310	F	F	F
3.2687334790595370	5.4959629088694779	12.4570974021264291	F	F	F
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14.5986804710254070	7.3279502039531375	11.2875453513566022	F	F	F
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Oxide reference: ZrO2(101)/fcc(100)_7x4/Pd E_tot= -2067.44534216 eV
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10.2275294632316065	3.7654931163417893	14.2435598356644064	T	T	T
12.5963557595765696	3.9073785630679283	14.8499468597399922	T	T	T
7.3307183223357502	5.4959628016039668	11.8723227294208407	F	F	F
11.7425013958488798	5.7130313253202649	15.3998326009474624	T	T	T
8.0393463944483479	3.5040042622809309	15.7554055371463928	T	T	T
9.5780216549781603	5.3846248755018014	16.8154691603455433	T	T	T
12.2116150400548253	3.9393676384664760	17.1406407157336673	T	T	T
8.2705044969295951	3.2852626633953173	17.8168425071876122	T	T	T
9.3906977239273139	5.6288112229262222	14.7825866015038123	T	T	T
7.3096217756178241	5.1932235159272127	18.3710029482382815	T	T	T
10.0722273457789218	3.2601425104440436	18.7524518333941721	T	T	T
11.4323851357659283	5.8411272034141497	17.6682276713533923	T	T	T
9.7931136977873763	9.1599375816511888	8.0000000000000000	F	F	F
12.5363102930756476	7.3279500263789501	8.3161459287561925	F	F	F
8.4743255254208680	7.3279501343428608	8.9009207394719176	F	F	F
7.6183192060923934	9.1599377071619443	9.4856979795260195	F	F	F
10.3615158793226616	7.3279501902136106	9.8018440286466415	F	F	F
11.8554838757371375	9.1599377592253770	10.9713994226004097	F	F	F
8.1867242632587391	7.3279502039531375	11.2875453513566022	F	F	F
10.5366957033706328	7.3279503119170482	11.8723201620723273	F	F	F
11.6803040493686083	9.1599375998964341	8.9009233068204310	F	F	F
9.6806893840421591	9.1599378847361308	12.4570974021264291	F	F	F
12.4238860572724263	7.3279503677877980	12.7732434512470512	F	F	F
7.5003430158814695	9.1490647151816074	13.9250610124788796	T	T	T
10.2278028864834702	7.4303486469995175	14.2444343271003167	T	T	T
12.5944353798082513	7.5695952065661549	14.8508760796837205	T	T	T
7.3307180195517043	9.1599377774706188	11.8723227294208407	F	F	F
11.7447048942136973	9.3774963227346060	15.4010079700964457	T	T	T

8.0372558093282844	7.1693256051692478	15.7553192276881493	T	T	T
9.5800805372534352	9.0491759653700683	16.8167896962230508	T	T	T
12.2024628670665543	7.5998700626881890	17.1415764406315674	T	T	T
8.2642163253997722	6.9512502582824514	17.8167950795596326	T	T	T
9.3900979206308843	9.2929684398090924	14.7844517041182044	T	T	T
7.3118901936122365	8.8590620111732648	18.3715473136329273	T	T	T
10.0625217343864328	6.9172888779621369	18.7562432192029824	T	T	T
11.4377712325618326	9.5065520066799145	17.6667687285731390	T	T	T
16.2050705111221340	1.8319876299178814	8.0000000000000000	F	F	F
18.9482671064104053	0.0000000746456413	8.3161459287561925	F	F	F
14.8862823387556311	0.0000001826095522	8.9009207394719176	F	F	F
14.0302760194271556	1.8319877554286361	9.4856979795260195	F	F	F
16.7734726926574247	0.0000002384803027	9.8018440286466415	F	F	F
18.2674406890718970	1.8319878074920686	10.9713994226004097	F	F	F
14.5986810765935022	0.0000002522198290	11.2875453513566022	F	F	F
16.9486525167053905	0.0000003601837396	11.8723201620723273	F	F	F
18.0922608627033661	1.8319876481631248	8.9009233068204310	F	F	F
16.0926461973769186	1.8319879330028237	12.4570974021264291	F	F	F
18.8358428706071841	0.0000004160544901	12.7732434512470512	F	F	F
13.9144107403073143	1.8711987336520199	13.9223242666348153	T	T	T
16.6414886320816180	-0.0373241603522708	14.2417455025275874	T	T	T
19.0103569271844357	-0.1053751949851718	14.8481413227564527	T	T	T
13.7426748328864665	1.8319878257373117	11.8723227294208407	F	F	F
18.1485788064088212	1.7440290508409397	15.4002462030740972	T	T	T
14.4547810501113467	0.1994719341994125	15.7543281814637091	T	T	T
15.9831652666884221	2.0257164745990934	16.8191411470088212	T	T	T
18.6372967849943869	-0.1004539880321128	17.1193246994135286	T	T	T
14.7112085483389379	0.3589589091537169	17.8136927527655793	T	T	T
15.8016793033321221	1.7648102536798158	14.7814746993352095	T	T	T
13.7445890372138511	2.1282261915498100	18.3671027797526420	T	T	T
16.5204568699598937	0.4441585316142921	18.7216929372313423	T	T	T
17.8495342379639794	1.6504715446017737	17.6578479988698973	T	T	T
16.2050702083380855	5.4959626057845350	8.0000000000000000	F	F	F
18.9482668036263568	3.6639750505122959	8.3161459287561925	F	F	F
14.8862820359715826	3.6639751584762061	8.9009207394719176	F	F	F
14.0302757166431071	5.4959627312952906	9.4856979795260195	F	F	F
16.7734723898733797	3.6639752143469568	9.8018440286466415	F	F	F
18.2674403862878485	5.4959627833587223	10.9713994226004097	F	F	F
14.5986807738094519	3.6639752280864832	11.2875453513566022	F	F	F
16.9486522139213456	3.6639753360503935	11.8723201620723273	F	F	F
18.0922605599193211	5.4959626240297785	8.9009233068204310	F	F	F
16.0926458945928736	5.4959629088694779	12.4570974021264291	F	F	F
18.8358425678231391	3.6639753919211442	12.7732434512470512	F	F	F
13.9140286682784993	5.5370208688520819	13.9230193887054217	T	T	T
16.6409019721787068	3.6263239608191209	14.2403046930538277	T	T	T
19.0111665645749071	3.5601731603073330	14.8491199255990232	T	T	T
13.7426745301024180	5.4959628016039668	11.8723227294208407	F	F	F
18.1453583190583387	5.4083447202760428	15.3978044408429717	T	T	T
14.4553354970112604	3.8646167459197089	15.7540794409066773	T	T	T
15.9817873458642108	5.6922851200435574	16.8179670638075365	T	T	T
18.6326364942433216	3.5659326711270931	17.1190125715832515	T	T	T
14.7062389172772825	4.0253147843370503	17.8141734515421248	T	T	T
15.8028588119827891	5.4282022598767226	14.7797590858178474	T	T	T
13.7453900603525252	5.7944361859907039	18.3692505614483252	T	T	T
16.5157887353105579	4.1099868843153047	18.7219146033054322	T	T	T
17.8446282542931272	5.3155501443456146	17.6586059447069879	T	T	T
16.2050699055540370	9.1599375816511888	8.0000000000000000	F	F	F
18.9482665008423083	7.3279500263789501	8.3161459287561925	F	F	F
14.8862817331875359	7.3279501343428608	8.9009207394719176	F	F	F
14.0302754138590604	9.1599377071619443	9.4856979795260195	F	F	F
16.7734720870893312	7.3279501902136106	9.8018440286466415	F	F	F
18.2674400835038035	9.1599377592253770	10.9713994226004097	F	F	F
14.5986804710254070	7.3279502039531375	11.2875453513566022	F	F	F

```
 16.9486519111372971  7.3279503119170482 11.8723201620723273   F   F   F
 18.0922602571352726  9.1599375998964341  8.9009233068204310   F   F   F
 16.0926455918088251  9.1599378847361308 12.4570974021264291   F   F   F
 18.8358422650390906  7.3279503677877980 12.7732434512470512   F   F   F
 13.9136123649500547  9.1993365668686327 13.9222923283906184   T   T   T
 16.6389178388351908  7.2917771063042167 14.2419358091136186   T   T   T
 19.0120822340734215  7.2226180221183451 14.8489254978661265   T   T   T
 13.7426742273183713  9.1599377774706188 11.8723227294208407   F   F   F
 18.1482339071278105  9.0709912821294125 15.4011668195091218   T   T   T
 14.4516168829111660  7.5323415707893666 15.7583479748417936   T   T   T
 15.9846355936207374  9.3567482637329409 16.8211747835487522   T   T   T
 18.6390278658334125  7.2256219800903461 17.1183087528486659   T   T   T
 14.7101795074444084  7.6872570649303809 17.8161451318418429   T   T   T
 15.8002710660951227  9.0937181045439086 14.7829421311271023   T   T   T
 13.7450680835956316  9.4560424450668172 18.3672153689465389   T   T   T
 16.5229502889318134  7.7675025276053828 18.7194977908145184   T   T   T
 17.8515792026317079  8.9766975618440217 17.6574015584224355   T   T   T

Metal reference: ZrO2(101)/fcc(100)_7x4/Pd E_tot= -426.19571974 eV
 D3-zero damping= -28.5402612 eV, D3-BJ damping= -34.8687026 eV
Pd
 1.0000000000000000
    19.2358686233000036    0.0000000000000000    0.0000000000000000
     0.0000000000000000   10.9919249276000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9359299014895974
  84
Cartesian
 -0.0000003968045556  0.0000000957804100  8.0189581111940207
  1.3738757433927569  1.3743329647165665  9.9727413401738563
  0.0000004241703870  0.0000000136829157 11.9265727826578303
  0.0000003694387242  2.7479805340712993  8.0178787137401351
  1.3738762793086055  4.1216301969121307  9.9727425032216921
 -0.0000006567799541  2.7479817655337131 11.9284369164005035
 -0.0000002326095671  5.4959626143120737  8.0189572572932128
  1.3738759646015442  6.8702949839703855  9.9727407791743126
  0.0000000547316628  5.4959638320915714 11.9265718745234341
 -0.0000000684145786  8.2439427242129852  8.0178796137516599
  1.3738755267482414  9.6175921818100907  9.9727417346962746
 -0.0000004652191342  8.2439434767733495 11.9284352150110493
  2.7495393665050938 -0.0000005199507970  8.0190904439889934
  4.1230925598397912  1.3748862670059143  9.9734318640059190
  2.7484836706869507 -0.0000010809503411 11.9276603753880313
  2.7477358180451934  2.7479804930225518  8.0203584112365256
  4.1230924093277181  4.1210772640615110  9.9734330614096063
  2.7478876325202850  2.7479817792166288 11.9265903785878038
  2.7495393528221781  5.4959630521653766  8.0190898774294173
  4.1230911504994729  6.8708493465371223  9.9734324574332334
  2.7484841562818842  5.4959612323375868 11.9276606534570853
  2.7477368168980405  8.2439442156507976  8.0203596803896087
  4.1230919030598372  9.6170377848874793  9.9734323139112018
  2.7478890418606032  8.2439436546512539 11.9265903788849510
  5.4947556754137006  0.0000001778779042  8.0182901437967811
  6.8700133399488044  1.3737817480387844  9.9732310407382609
  5.4940053384367840 -0.0000005336337127 11.9284538522591301
  5.4958293814758079  2.7479810540220959  8.0186180921366610
  6.8700145850941343  4.1221806540395196  9.9732310314660833
  5.4974630168047929  2.7479815602899773 11.9268263054863670
  5.4947550733654094  5.4959623680195904  8.0182899865918333
  6.8700132578513102  6.8697445265458494  9.9732308195294728
  5.4940052152905432  5.4959623543366751 11.9284534883804376
  5.4958291625491569  8.2439436820170844  8.0186201169110394
  6.8700134767779621  9.6181437131949359  9.9732320850505936
  5.4974606359774585  8.2439438325291583 11.9268250165285252
```

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  8.2440665310122760 -0.0000002462924828  8.0187010625135304
  9.6179350094787015  1.3736330614719228  9.9729661328395469
  8.2431671533523811 -0.0000011219990883 11.9272344704793145
  8.2443640204316111  2.7479818202653759  8.0183631448022226
  9.6179345442595672  4.1223302917175992  9.9729669264486578
  8.2440258474664692  2.7479811634854219 11.9276626839656732
  8.2440671991930099  5.4959624911658320  8.0187011719768559
  9.6179341474550117  6.8695951421502830  9.9729666117415956
  8.2431677143519249  5.4959622859220962 11.9272363701224613
  8.2443653476744352  8.2439438872608211  8.0183621596322912
  9.6179347631862182  9.6182921671522195  9.9729676379602736
  8.2440268326364006  8.2439442156507976 11.9276633454535137
 10.9918022177161028  0.0000004652191342  8.0187008756605955
 12.3658555159607744  1.3737809817955047  9.9732300692512457
 10.9927021677763221 -0.0000003557558085 11.9272337430026436
 10.9915030977476622  2.7479806982662875  8.0183634228712961
 12.3658548318149872  4.1221809073220328  9.9732312436998605
 10.9918407370790909  2.7479816287045558 11.9276644400867706
 10.9918024890922812  5.4959620259466977  8.0187003624026918
 12.3658552149366283  6.8697448208771101  9.9732305892020428
 10.9927009773626541  5.4959620943612766 11.9272359272071977
 10.9915040829175936  8.2439431620662873  8.0183629806072343
 12.3658555022778582  9.6181436241074003  9.9732320099431409
 10.9918422148339889  8.2439431483833729 11.9276631139768092
 13.7411136320320786  0.0000000547316628  8.0182907732109037
 15.1127762600829900  1.3748869922004470  9.9734324437503172
 13.7418633532777825  0.0000002189266514 11.9284538726349396
 13.7400398701054556  2.7479815466070616  8.0186182674352828
 15.1127762600829900  4.1210750474291657  9.9734338463977608
 13.7384076452496515  2.7479817381678817 11.9268255719680383
 13.7411118669359524  5.4959622448733496  8.0182900867829829
 15.1127758632784346  6.8708494149517012  9.9734316861280146
 13.7418632985461198  5.4959628742874722 11.9284545637707478
 13.7400390092146285  8.2439439830412304  8.0186190281349621
 15.1127766107768391  9.6170377301558165  9.9734327877512925
 13.7384064822018157  8.2439430389200457 11.9268246549155190
 16.4863290652340808 -0.0000000273658314  8.0190905216757287
 17.8619928639421808  1.3743332794236280  9.9727410505504892
 16.4873835432727098 -0.0000003283899771 11.9276598964859808
 16.4881316695728195  2.7479810403391802  8.0203589848430425
 17.8619928502592664  4.1216299369367322  9.9727426263679337
 16.4879803613656080  2.7479805203883836 11.9265901873241305
 16.4863309261106181  5.4959627785070619  8.0190894794920009
 17.8619932333809039  6.8702956200773917  9.9727419969538111
 16.4873854725638260  5.4959629563849663 11.9276607858755028
 16.4881318748165562  8.2439434494075172  8.0203590188448501
 17.8619926176496975  9.6175921407613441  9.9727419125741790
 16.4879806487068379  8.2439438325291583 11.9265907835152447

Interface: ZrO2(101)/fcc(100)_7x4/Ir E_tot= -2799.18116166 eV
 D3-zero damping= -80.4583837 eV, D3-BJ damping= -96.0626133 eV
 O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr
O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr Ir
 1.0000000000000000
    19.0054425018500055    0.0000000000000000    0.0000000000000000
     0.0000000000000000   10.8602528582000026    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.4843427459152849
   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2   4   2
2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2   4
2   2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2
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4   2   2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4
2   4   2   2   1   2   1   4   2   4   2   4   2   2   1  84
Selective dynamics
Cartesian
  3.3406552640695582  1.8100422833170515  8.0000000000000018   F   F   F
  6.0509911570830459  0.0000000737514625  8.3161459287561943   F   F   F
  2.0376648313073069  0.0000001804220757  8.9009207394719194   F   F   F
  1.1919125961567956  1.8100424073243153  9.4856979795260212   F   F   F
  3.9022485661786139  0.0000002356235515  9.8018440286466468   F   F   F
  5.3783203470529601  1.8100424587640807 10.9713994226004115   F   F   F
  1.7535087394497764  0.0000002491984922 11.2875453513566040   F   F   F
  4.0753299142907080  0.0000003558691051 11.8723201620723291   F   F   F
  5.2052389966481023  1.8100423013437352  8.9009233068204328   F   F   F
  3.2295776791401969  1.8100425827713449 12.4570974021264309   F   F   F
  5.9399136491620155  0.0000004110705809 12.7732434512470530   F   F   F
  1.0727483573014329  1.8638138445186190 13.9568428484644613   T   T   T
  3.8153272114716628  0.0000117331280929 14.2489854887763503   T   T   T
  6.0866524319997808  0.0000225276476309 14.8508381080477658   T   T   T
  0.9077565790148355  1.8100424767907641 11.8723227294208460   F   F   F
  5.3486312695486546  1.8108067208160348 15.4746926673332919   T   T   T
  1.5727546643126578 -0.0000194428274378 15.6946795634069147   T   T   T
  3.2762405908817986  1.4632243760357286 16.8561074293019679   T   T   T
  5.9094425554218066 -0.0000257286840815 17.4189247057391370   T   T   T
  1.9755732618484776 -0.0000389695905044 17.7672569296494096   T   T   T
  2.9420542309727931  1.7786961722482504 14.8629410424979085   T   T   T
  0.8060779908173670  1.7346297458606117 17.9396177424437084   T   T   T
  3.7810804462121745  0.0000160343587407 19.0361171789514430   T   T   T
  4.9942975958822977  1.8095440525700248 17.9862464824892569   T   T   T
  3.3406549649125559  5.4301265693837060  8.0000000000000018   F   F   F
  6.0509908579260436  3.6200843598181178  8.3161459287561943   F   F   F
  2.0376645321503046  3.6200844664887302  8.9009207394719194   F   F   F
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Oxide reference: ZrO2(101)/fcc(100)_7x4/Ir E_tot= -2070.05398969 eV
 D3-zero damping= -30.4142084 eV, D3-BJ damping= -45.2198033 eV
 O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr
O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr
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2   4   2   2   1   2   1   4   2   4   2   4   2   2   1
Selective dynamics
Cartesian
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  2.0376648313073069  0.0000001804220757  8.9009207394719176   F   F   F
  1.1919125961567956  1.8100424073243153  9.4856979795260195   F   F   F
  3.9022485661786139  0.0000002356235515  9.8018440286466415   F   F   F
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  4.0753299142907080  0.0000003558691051 11.8723201620723273   F   F   F
  5.2052389966481023  1.8100423013437352  8.9009233068204310   F   F   F
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17.9300211044186213	1.8105056147582730	15.4706903407384502	T	T	T
14.3470787434203473	0.0002969848243013	15.7426797079067082	T	T	T
15.7749106604642719	1.8100521934449356	16.8815633480762592	T	T	T
18.5067424138168661	-0.0001260666042417	17.1506892356470964	T	T	T
14.5736957739434949	0.0007132791696235	17.8432961179368483	T	T	T
15.6111026685249854	1.8099832167504759	14.8210091340611925	T	T	T
13.6265377416359836	1.8107624782732148	18.4558592202074507	T	T	T
16.4342527602236750	0.0011554188397922	18.6791054345447307	T	T	T
17.6442646701885870	1.8097338746479783	17.7102502299282953	T	T	T
16.0109499661458905	5.4301265693837060	7.9999999999999991	F	F	F
18.7212858591593800	3.6200843598181178	8.3161459287561925	F	F	F
14.7079595333836419	3.6200844664887302	8.9009207394719176	F	F	F
13.8622072982331304	5.4301266933909700	9.4856979795260195	F	F	F
16.5725432682549538	3.6200845216902064	9.8018440286466415	F	F	F
18.0486150491292925	5.4301267448307353	10.9713994226004097	F	F	F
14.4238034415261112	3.6200845352651476	11.2875453513566022	F	F	F
16.7456246163670421	3.6200846419357600	11.8723201620723273	F	F	F
17.8755336987244391	5.4301265874103901	8.9009233068204310	F	F	F
15.8998723812165323	5.4301268688380002	12.4570974021264291	F	F	F
18.6102083512383487	3.6200846971372358	12.7732434512470512	F	F	F
13.7283583983140201	5.4301777039261134	13.9520900414838938	T	T	T
16.4741975709607047	3.6202144335926696	14.2517441925100457	T	T	T
18.8091270579402270	3.6201822467139553	14.8705700998858283	T	T	T

```
 13.5780512810911702  5.4301267628574204 11.8723227294208407   F   F   F
 17.9302743651144141  5.4300112412778896 15.4711444697097793   T   T   T
 14.3467816150390703  3.6194494082423847 15.7422380279016263   T   T   T
 15.7738606280435647  5.4305910410815157 16.8797083389070472   T   T   T
 18.5088437817501053  3.6200788849316039 17.1521622917426022   T   T   T
 14.5723653291695250  3.6209079097628951 17.8422820471137733   T   T   T
 15.6107715767452859  5.4301428761976362 14.8193308334960143   T   T   T
 13.6275100076412290  5.4309790893076455 18.4558015348144302   T   T   T
 16.4339624043264472  3.6226272032501616 18.6764454185264803   T   T   T
 17.6422570195009634  5.4294817573746856 17.7091008136767485   T   T   T
 16.0109496669888891  9.0502108554503611  7.9999999999999991   F   F   F
 18.7212855600023751  7.2401686458847729  8.3161459287561925   F   F   F
 14.7079592342266405  7.2401687525553866  8.9009207394719176   F   F   F
 13.8622069990761290  9.0502109794576260  9.4856979795260195   F   F   F
 16.5725429690979489  7.2401688077568611  9.8018440286466415   F   F   F
 18.0486147499722911  9.0502110308973904 10.9713994226004097   F   F   F
 14.4238031423691098  7.2401688213318023 11.2875453513566022   F   F   F
 16.7456243172100407  7.2401689280024151 11.8723201620723273   F   F   F
 17.8755333995674341  9.0502108734770452  8.9009233068204310   F   F   F
 15.8998720820595292  9.0502111549046536 12.4570974021264291   F   F   F
 18.6102080520813473  7.2401689832038905 12.7732434512470512   F   F   F
 13.7289407067591167  9.0506763856664296 13.9518242444791358   T   T   T
 16.4741889172496094  7.2400730377656632 14.2517772209734019   T   T   T
 18.8091624739670671  7.2398405671174366 14.8705880838555125   T   T   T
 13.5780509819341688  9.0502110489240728 11.8723227294208407   F   F   F
 17.9300484939713698  9.0495487614566557 15.4707075075298999   T   T   T
 14.3467829496902102  7.2413472237157812 15.7422644221072687   T   T   T
 15.7749728654656884  9.0512324360635485 16.8816025510688164   T   T   T
 18.5088677760810896  7.2398484074098697 17.1521399854812167   T   T   T
 14.5723674020412357  7.2406270672099415 17.8422843618215907   T   T   T
 15.6110982405790395  9.0503169818343903 14.8210744425069016   T   T   T
 13.6265783232054307  9.0512275322514189 18.4558384494315995   T   T   T
 16.4339818510198157  7.2396911563851116 18.6763877416339632   T   T   T
 17.6443927709969195  9.0492735673602347 17.7102162153692611   T   T   T

Metal reference: ZrO2(101)/fcc(100)_7x4/Ir E_tot= -704.09340653 eV
 D3-zero damping= -34.7532889 eV, D3-BJ damping= -37.6665635 eV
Ir
 1.0000000000000000
    19.0054425018500055    0.0000000000000000    0.0000000000000000
     0.0000000000000000   10.8602528582000026    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7037057660956023
  84
Cartesian
  0.0000000000000000  0.0000000000000000  7.9998738643110467
  1.3576197342432688  1.3575268518811154  9.8513007229798824
  0.0000000000000000  0.0000000000000000 11.7027246893708590
  0.0000000000000000  2.7150632145500007  7.9998075754559181
  1.3576197699596688  4.0725995628487714  9.8513007373499963
  0.0000000000000000  2.7150632145500007 11.7027749356606918
  0.0000000000000000  5.4301264291000013  7.9998738752532672
  1.3576197582910190  6.7876533033864002  9.8513007373499963
 -0.0000000000000000  5.4301264291000013 11.7027246893708590
 -0.0000000000000000  8.1451896436500029  7.9998075702899607
  1.3576197699596688  9.5027259839136011  9.8513007361810061
 -0.0000000000000000  8.1451896436500029 11.7027749500308058
  2.7150282645247446 -0.0000000000000000  7.9997250976191712
  4.0725539914041677  1.3576951481105271  9.8513307251775402
  2.7150447548688184  0.0000000000000000 11.7028707320070584
  2.7151851089002026  2.7150632145500007  7.9996770647164874
  4.0725539914041677  4.0724312809894778  9.8513307395476541
  2.7152418811503320  2.7150632145500007 11.7029360046221846
  2.7150282645247446  5.4301264291000013  7.9997251281696169
```

4.0725539593212483	6.7878216129269253	9.8513307395476541
2.7150447548688184	5.4301264291000013	11.7028707320070584
2.7151851089002026	8.1451896436500029	7.9996770607504351
4.0725539593212483	9.5025576996854060	9.8513307251775402
2.7152418811503320	8.1451896436500029	11.7029359965076019
5.4301243043530967	0.0000000000000000	7.9996774708812932
6.7876273921964518	1.3575694864957226	9.8512150820178146
5.4302386784353756	-0.0000000000000000	11.7028092569658462
5.4301084828721109	2.7150632145500007	7.9995768883088818
6.7876273921964518	4.0725569426042822	9.8512150843867143
5.4301812558498055	2.7150632145500007	11.7029054406405724
5.4301243043530967	5.4301264291000013	7.9996774885940951
6.7876274255439562	6.7876958670416805	9.8512150843867143
5.4302386784353756	5.4301264291000013	11.7028092679080640
5.4301084828721109	8.1451896436500029	7.9995768883088818
6.7876274255439562	9.5026833845419141	9.8512150795842430
5.4301812201334059	8.1451896436500029	11.7029054442740534
8.1450155450568342	0.0000000000000000	7.9996744155760950
9.5027212509250027	1.3575655033838780	9.8512075087005258
8.1450818290503655	0.0000000000000000	11.7027138849502101
8.1451210363400328	2.7150632145500007	7.9996124369570687
9.5027212509250027	4.0725609389172464	9.8512074753530179
8.1451685742419961	2.7150632145500007	11.7027887967072068
8.1450155450568342	5.4301264291000013	7.9996743987724059
9.5027212509250027	6.7876919173873391	9.8512074870216697
8.1450818162127252	5.4301264291000013	11.7027138860397866
8.1451210387736044	8.1451896436500029	7.9996124622694023
9.5027212509250027	9.5026873699126693	9.8512075087005258
8.1451685518367150	8.1451896436500029	11.7027888239149576
10.8604269567931713	0.0000000000000000	7.9996744298667988
12.2178150895071767	1.3575694379416829	9.8512151199931193
10.8603606727996400	-0.0000000000000000	11.7027138977878487
10.8603214655099727	2.7150632145500007	7.9996124512477831
12.2178150872482725	4.0725569783206828	9.8512150960553626
10.8602739371756520	2.7150632145500007	11.7027888348571789
10.8604269567931713	5.4301264291000013	7.9996744131425199
12.2178150895071767	6.7876959004991813	9.8512150843867143
10.8603606856372803	5.4301264291000013	11.7027138753825692
10.8603214630764011	8.1451896436500029	7.9996124621900035
12.2178150751370591	9.5026833845419141	9.8512150820178146
10.8602739276080094	8.1451896436500029	11.7027887739078569
13.5753181832062033	0.0000000000000000	7.9996774837189317
14.9328885425287510	1.3576951614216448	9.8513307347451828
13.5752037973758668	-0.0000000000000000	11.7028092822781833
13.5753340404035860	2.7150632145500007	7.9995768919423647
14.9328885201234680	4.0724312452730773	9.8513307251775402
13.5752612817165961	2.7150632145500007	11.7029054644204358
13.5753181832062033	5.4301264291000013	7.9996774805589297
14.9328885104458315	6.7878215876145909	9.8513307395476541
13.5752038105769888	5.4301264291000013	11.7028092593994231
13.5753340175248276	8.1451896436500029	7.9995769096551683
14.9328885068123522	9.5025576887431864	9.8513307395476541
13.5752612460001973	8.1451896436500029	11.7029054442740534
16.2904142373252654	0.0000000000000000	7.9997251080232328
17.6478227318903436	1.3575268518811154	9.8513007361810061
16.2903977469811885	0.0000000000000000	11.7028707297481542
16.2902573929498082	2.7150632145500007	7.9996770743147101
17.6478227318903436	4.0725995628487714	9.8513007373499963
16.2902006206996717	2.7150632145500007	11.7029360046221846
16.2904142373252654	5.4301264291000013	7.9997251189654577
17.6478227318903436	6.7876532688699083	9.8513007148347196
16.2903977469811885	5.4301264291000013	11.7028707140828718
16.2902573929498082	8.1451896436500029	7.9996770607504315

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 17.6478227318903436  9.5027259946502323  9.8513007505511201
 16.2902006206996717  8.1451896436500029 11.7029359965076019

Interface: ZrO2(101)/fcc(100)_7x4/Rh E_tot= -2676.26156011 eV
 D3-zero damping= -74.6999093 eV, D3-BJ damping= -92.2394334 eV
 O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr
O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr Rh
 1.0000000000000000
    18.7436388669600049    0.0000000000000000    0.0000000000000000
     0.0000000000000000   10.7106507811200018    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.5198948638977186
   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2   4   2
2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2   4
2   2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2
4   2   2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4
2   4   2   2   1   2   1   4   2   4   2   4   2   2   1  84
Selective dynamics
Cartesian
  3.2946370936974296  1.7851086018712825  8.0000000000000000   F   F   F
  5.9676375872065552  0.0000000727355219  8.3161459287561925   F   F   F
  2.0095956053752171  0.0000001779367268  8.9009207394719176   F   F   F
  1.1754937703328427  1.7851087241703223  9.4856979795260195   F   F   F
  3.8484943397894935  0.0000002323777916  9.8018440286466451   F   F   F
  5.3042329472818546  1.7851087749014951 10.9713994226004097   F   F   F
  1.7293538184709754  0.0000002457657350 11.2875453513566022   F   F   F
  4.0191914589596411  0.0000003509669396 11.8723201620723273   F   F   F
  5.1335358258505268  1.7851086196496453  8.9009233068204310   F   F   F
  3.1850896239172672  1.7851088972005353 12.4570974021264291   F   F   F
  5.8580901933739185  0.0000004054080044 12.7732434512470512   F   F   F
  1.0680670778542840  1.7674884643447029 13.9992159364252124   T   T   T
  3.7464559511360878 -0.0000038296204838 14.3099034939184886   T   T   T
  5.9592492765505396  0.0000258446461085 14.8421104357482836   T   T   T
  0.8952520571149502  1.7851087926798577 11.8723227294208442   F   F   F
  5.1720574110488577  1.7858300658848438 15.5163945761792554   T   T   T
  1.6623391924739332 -0.0000217003247675 15.8332181584542102   T   T   T
  3.0535520747865412  1.7510333025596503 17.1230038347728666   T   T   T
  5.7527526733005914 -0.0000045642042934 17.6151710880347636   T   T   T
  1.7525854604395950 -0.0000471064530737 17.9164841436034052   T   T   T
  2.9415679653179660  1.7785070317239566 15.0262767903042764   T   T   T
  0.7692772403983312  1.8384846511513220 18.5441320265245544   T   T   T
  3.5505848962208382  0.0000136614101590 18.9812023357571960   T   T   T
  4.9134541377584773  1.8069258375203052 18.3201693975745989   T   T   T
  3.2946367986613727  5.3553255289112700  8.0000000000000000   F   F   F
  5.9676372921704974  3.5702169997755102  8.3161459287561925   F   F   F
  2.0095953103391602  3.5702171049767144  8.9009207394719176   F   F   F
  1.1754934752967856  5.3553256512103102  9.4856979795260195   F   F   F
  3.8484940447534370  3.5702171594177794  9.8018440286466451   F   F   F
  5.3042326522457977  5.3553257019414824 10.9713994226004097   F   F   F
  1.7293535234349184  3.5702171728057230 11.2875453513566022   F   F   F
  4.0191911639235851  3.5702172780069272 11.8723201620723273   F   F   F
  5.1335355308144699  5.3553255466896328  8.9009233068204310   F   F   F
  3.1850893288812103  5.3553258242405235 12.4570974021264291   F   F   F
  5.8580898983378606  3.5702173324479922 12.7732434512470512   F   F   F
  1.1109479741893267  5.3553232787091902 13.9941678487017516   T   T   T
  3.7444984335433191  3.5629936191053067 14.3145619062443021   T   T   T
  5.9718470957416807  3.5763861470016294 14.8354010863344676   T   T   T
  0.8952517620788932  5.3553257197198461 11.8723227294208442   F   F   F
  5.1574762386101076  5.3553406213248813 15.4675428769139884   T   T   T
  1.6577219411651569  3.5641404557528484 15.8277437314584475   T   T   T
  3.0656749280683799  5.3553177348344105 17.1554865383293205   T   T   T
  5.6866827458382865  3.5925729858617252 17.5745105519917679   T   T   T
```

1.7263211823654983	3.5773982177004213	17.8801018034404748	T	T	T
2.9619213598261589	5.3553216197522335	15.0233646915896841	T	T	T
0.8683542566253909	5.3552665887256081	18.6851967403140407	T	T	T
3.4373888306726519	3.4577204065501417	19.0057947713072224	T	T	T
4.9100643219947271	5.3553842695324088	18.3491053316751369	T	T	T
3.2946365036253162	8.9255424559512591	8.0000000000000000	F	F	F
5.9676369971344414	7.1404339268154988	8.3161459287561925	F	F	F
2.0095950153031032	7.1404340320167030	8.9009207394719176	F	F	F
1.1754931802607289	8.9255425782502975	9.4856979795260195	F	F	F
3.8484937497173797	7.1404340864577671	9.8018440286466451	F	F	F
5.3042323572097407	8.9255426289814714	10.9713994226004097	F	F	F
1.7293532283988617	7.1404340998457112	11.2875453513566022	F	F	F
4.0191908688875282	7.1404342050469154	11.8723201620723273	F	F	F
5.1335352357784139	8.9255424737296227	8.9009233068204310	F	F	F
3.1850890338451543	8.9255427512805117	12.4570974021264291	F	F	F
5.8580896033018028	7.1404342594879804	12.7732434512470512	F	F	F
1.0680747958798544	8.9431403887407281	13.9992222004277451	T	T	T
3.7444921140277252	7.1476698941306980	14.3145757018873976	T	T	T
5.9718487522977766	7.1342897891601877	14.8354176530529376	T	T	T
0.8952514670428363	8.9255426467598333	11.8723227294208442	F	F	F
5.1720593267893609	8.9248499991733539	15.5164264282142721	T	T	T
1.6576867220877667	7.1464736652975036	15.8277704558080963	T	T	T
3.0535487205747764	8.9595682916465904	17.1230377112063188	T	T	T
5.6866682938349351	7.1181578160601591	17.5744997930229410	T	T	T
1.7262921825112103	7.1331647108025571	17.8801762258105477	T	T	T
2.9415560108839442	8.9321591863403800	15.0262903216936721	T	T	T
0.7692821084355279	8.8720895910996447	18.5442500211462686	T	T	T
3.4373089823361034	7.2528346258635006	19.0059235849269648	T	T	T
4.9133841389832256	8.9037906592193412	18.3200682807664030	T	T	T
9.5425167160174311	1.7851086018712825	8.0000000000000000	F	F	F
12.2155172095265598	0.0000000727355219	8.3161459287561925	F	F	F
8.2574752276952204	0.0000001779367268	8.9009207394719176	F	F	F
7.4233733926528460	1.7851087241703223	9.4856979795260195	F	F	F
10.0963739621094959	0.0000002323777916	9.8018440286466451	F	F	F
11.5521125696018583	1.7851087749014951	10.9713994226004097	F	F	F
7.9772334407909771	0.0000002457657350	11.2875453513566022	F	F	F
10.2670710812796457	0.0000003509669396	11.8723201620723273	F	F	F
11.3814154481705323	1.7851086196496453	8.9009233068204310	F	F	F
9.4329692462372705	1.7851088972005353	12.4570974021264291	F	F	F
12.1059698156939177	0.0000004054080044	12.7732434512470512	F	F	F
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Oxide reference: ZrO2(101)/fcc(100)_7x4/Rh E_tot= -2072.1002207 eV
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O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
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Selective dynamics
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Metal reference: ZrO2(101)/fcc(100)_7x4/Rh E_tot= -580.15073117 eV
 D3-zero damping= -28.0589916 eV, D3-BJ damping= -33.8381026 eV
Rh
 1.0000000000000000
    18.7436388669600049    0.0000000000000000    0.0000000000000000
     0.0000000000000000   10.7106507811200018    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.6867355476600920
  84
Cartesian
  0.0000000000000000  0.0000000000000000  8.0018641931804950
  1.3382859300030334  1.3400478182555671  9.8435701976826238
 -0.0000000000000000 -0.0000000000000000 11.6845179222141073
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0.0000000000000000	2.6776626952800004	8.0000126714285713
1.3382858847691652	4.0152775982753113	9.8435701976826238
-0.0000000000000000	2.6776626952800004	11.6868202333743820
-0.0000000000000000	5.3553253905600009	8.0018640716731166
1.3382859436194070	6.6953731487747881	9.8435702180052207
-0.0000000000000000	5.3553253905600009	11.6845179753785366
-0.0000000000000000	8.0329880858400013	8.0000128170633733
1.3382859745769422	9.3706030218456071	9.8435701976826238
0.0000000000000000	8.0329880858400013	11.6868201529756419
2.6744498114905508	-0.0000000000000000	8.0013434866669915
4.0143184758035853	1.3383935502313626	9.8438718296492222
2.6744147577964559	-0.0000000000000000	11.6865539593316861
2.6782867906033192	2.6776626952800004	8.0012603458034111
4.0143184044679128	4.0169318403286409	9.8438718499718210
2.6781321388159292	2.6776626952800004	11.6855932548262231
2.6744497187186695	5.3553253905600009	8.0013434747253047
4.0143184498327082	6.6937189098338266	9.8438718769290485
2.6744147318255780	5.3553253905600009	11.6865539298876691
2.6782868833751992	8.0329880858400013	8.0012604082987604
4.0143185097425578	9.3722572618461744	9.8438718914837633
2.6781321388159292	8.0329880858400013	11.6855933654837685
5.3533695748939669	0.0000000000000000	8.0017272907885353
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5.3531946870525049	-0.0000000000000000	11.6861059344926002
5.3560928382246704	2.6776626952800004	8.0036158441131366
6.6941238516452168	4.0164239403652493	9.8438948400752331
5.3553102357870026	2.6776626952800004	11.6843937084763674
5.3533695479367411	5.3553253905600009	8.0017274556813831
6.6941238516452168	6.6942268677119783	9.8438948854400277
5.3531946542001263	5.3553253905600009	11.6861059112562753
5.3560928382246704	8.0329880858400013	8.0036158132036270
6.6941238786024435	9.3717493445416284	9.8438948197526273
5.3553102357870026	8.0329880858400013	11.6843938042835056
8.0323306488387942	-0.0000000000000000	8.0017497158600079
9.3718194334800025	1.3404209579394049	9.8433795320900828
8.0326142543754901	-0.0000000000000000	11.6858590010098808
8.0323292998568903	2.6776626952800004	8.0011399950789173
9.3718194334800025	4.0149044056633638	9.8433794105338830
8.0328161769056372	2.6776626952800004	11.6861542008432426
8.0323306488387942	5.3553253905600009	8.0017498553378097
9.3718194334800025	6.6957464015584414	9.8433795320900828
8.0326142543754901	5.3553253905600009	11.6858589496226681
8.0323292998568903	8.0329880858400013	8.0011399187108605
9.3718194334800025	9.3702297921015134	9.8433793969175074
8.0328161911913512	8.0329880858400013	11.6861542075770473
10.7113081728873407	0.0000000000000000	8.0017497680756264
12.0495149707502502	1.3389014646020103	9.8438947887950921
10.7110246125845130	0.0000000000000000	11.6858589363917389
10.7113095671031129	2.6776626952800004	8.0011399535329097
12.0495150154457153	4.0164239403652493	9.8438947628242151
10.7108226901759132	2.6776626952800004	11.6861541592250990
10.7113081728873407	5.3553253905600009	8.0017497425026693
12.0495149707502502	6.6942268068157729	9.8438948091176979
10.7110246125845130	5.3553253905600009	11.6858589342665464
10.7113095671031129	8.0329880858400013	8.0011399284926572
12.0495149295073105	9.3717493504569678	9.8438947831468209
10.7108227210025220	8.0329880858400013	11.6861542075770473
13.3902692852325469	0.0000000000000000	8.0017274240641516
14.7293204420385742	1.3383936120457078	9.8438718769290485
13.3904441345426957	0.0000000000000000	11.6861058340494424
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14.7293204499893360	4.0169318403286409	9.8438718499718210
13.3883286311730032	2.6776626952800004	11.6843937865452752

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 13.3902693190232629  5.3553253905600009  8.0017272889567632
 14.7293203911564223  6.6937188751039605  9.8438718499718210
 13.3904442013437013  5.3553253905600009 11.6861059277971737
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 14.7293203572174516  9.3722572965760325  9.8438718499718210
 13.3883286311730032  8.0329880858400013 11.6843937065066985
 16.0691891279187153  0.0000000000000000  8.0013435836216384
 17.4053529233405797  1.3400478452127937  9.8435702322909346
 16.0692241091635637 -0.0000000000000000 11.6865538991427655
 16.0653520763566817  2.6776626952800004  8.0012602911157487
 17.4053529233405797  4.0152775723044343  9.8435702325599213
 16.0655067281440651  2.6776626952800004 11.6855934279674578
 16.0691891482413141  5.3553253905600009  8.0013434254415490
 17.4053529233405797  6.6953731035409199  9.8435702045161051
 16.0692241351344407  5.3553253905600009 11.6865540165569044
 16.0653519835848044  8.0329880858400013  8.0012604111969345
 17.4053529233405797  9.3706030335307684  9.8435702045161051
 16.0655067145276895  8.0329880858400013 11.6855931991970277

Interface: ZrO2(101)/fcc(100)_7x4/Ru E_tot= -2817.53139885 eV
 D3-zero damping= -73.2903613 eV, D3-BJ damping= -90.7268189 eV
 O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr
O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O
Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr Ru
 1.0000000000000000
    18.6633631935800040    0.0000000000000000    0.0000000000000000
     0.0000000000000000   10.6647789677600020    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.7789086672896843
   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2   4   2
2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2   4
2   2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4   2
4   2   2   1   2   1   4   2   4   2   4   2   2   1   2   1   4   2   4
2   4   2   2   1   2   1   4   2   4   2   4   2   2   1  84
Selective dynamics
Cartesian
  3.2805267486829672  1.7774632990520820  7.9999999999999991   F   F   F
  5.9420792562335194  0.0000000724240086  8.3161459287561925   F   F   F
  2.0009888646250333  0.0000001771746555  8.9009207394719176   F   F   F
  1.1704593394714049  1.7774634208273368  9.4856979795260195   F   F   F
  3.8320119226442131  0.0000002313825588  9.8018440286466415   F   F   F
  5.2815158604541725  1.7774634713412369 10.9713994226004097   F   F   F
  1.7219473034780544  0.0000002447131640 11.2875453513566022   F   F   F
  4.0019779763962386  0.0000003494638106 11.8723201620723273   F   F   F
  5.1115498044506520  1.7774633167543032  8.9009233068204310   F   F   F
  3.1714484512426102  1.7774635931164922 12.4570974021264291   F   F   F
  5.8330010344154184  0.0000004036717139 12.7732434512470512   F   F   F
  1.1103217037188478  1.8060597672535794 14.0182295323151838   T   T   T
  3.7218587458300205  0.0162484944180823 14.3595350286379144   T   T   T
  5.9201475992806918 -0.0152460642355989 14.8232225342643300   T   T   T
  0.8914178516951895  1.7774634890434580 11.8723227294208407   F   F   F
  5.1457956270365930  1.7709543214946888 15.5763820903650245   T   T   T
  1.6523498453079104  0.0672350815575541 15.9053448446070593   T   T   T
  3.0785766902645064  1.8224348694854446 17.3387974859583878   T   T   T
  5.7619207215081349 -0.0698942235113788 17.7357796997797017   T   T   T
  1.7600261744314318 -0.0284296363298685 17.9642195613078499   T   T   T
  2.9510271792372826  1.7906932648389902 15.1605779316216402   T   T   T
  0.8168295081694430  1.7809228053544099 18.7446745691619476   T   T   T
  3.5475799072684118 -0.0533462415102585 19.1360245775709146   T   T   T
  4.9573544632787589  1.6406605532724907 18.5221178282361123   T   T   T
  3.2805264549104973  5.3323896216387361  7.9999999999999991   F   F   F
  5.9420789624610491  3.5549263950106638  8.3161459287561925   F   F   F
  2.0009885708525639  3.5549264997613097  8.9009207394719176   F   F   F
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1.1704590456989350	5.3323897434139917	9.4856979795260195	F	F	F
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5.2815155666817031	5.3323897939278915	10.9713994226004097	F	F	F
1.7219470097055845	3.5549265672998192	11.2875453513566022	F	F	F
4.0019776826237692	3.5549266720504651	11.8723201620723273	F	F	F
5.1115495106781816	5.3323896393409580	8.9009233068204310	F	F	F
3.1714481574701403	5.3323899157031471	12.4570974021264291	F	F	F
5.8330007406429480	3.5549267262583686	12.7732434512470512	F	F	F
1.0893241630230983	5.3195554097542672	14.0154809151698743	T	T	T
3.7228985022041510	3.5483070301900730	14.3602695594778620	T	T	T
5.9241942011911686	3.5608994903358711	14.8216018249970229	T	T	T
0.8914175579227196	5.3323898116301134	11.8723227294208407	F	F	F
5.1428679225640908	5.3262121079019691	15.5275850546791450	T	T	T
1.6513733648363687	3.5496882016175060	15.9171276444302592	T	T	T
3.0681117287838813	5.3858751274789967	17.2227211928885851	T	T	T
5.5588415967483487	3.5168060483936285	17.8605047059080455	T	T	T
1.6499719238637969	3.5472154916172056	17.9880996064186469	T	T	T
2.9357533451981399	5.3369434889523424	15.1022991944180944	T	T	T
0.7488021665664449	5.3674739516578036	18.5862917500735989	T	T	T
3.1651966189145080	3.9622064136745090	19.3565315149436508	T	T	T
4.8427111042677300	5.3046769638489195	18.5408425711184961	T	T	T
3.2805261611380279	8.8873159442253922	7.9999999999999991	F	F	F
5.9420786686885796	7.1098527175973194	8.3161459287561925	F	F	F
2.0009882770800940	7.1098528223479658	8.9009207394719176	F	F	F
1.1704587519264651	8.8873160660006469	9.4856979795260195	F	F	F
3.8320113350992733	7.1098528765558680	9.8018440286466415	F	F	F
5.2815152729092336	8.8873161165145458	10.9713994226004097	F	F	F
1.7219467159331148	7.1098528898864739	11.2875453513566022	F	F	F
4.0019773888512997	7.1098529946371203	11.8723201620723273	F	F	F
5.1115492169057131	8.8873159619276141	8.9009233068204310	F	F	F
3.1714478636976708	8.8873162382898006	12.4570974021264291	F	F	F
5.8330004468704768	7.1098530488450233	12.7732434512470512	F	F	F
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0.8914172641502497	8.8873161342167659	11.8723227294208407	F	F	F
5.1440159249409785	8.8753806007086578	15.5118196195102733	T	T	T
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3.0306621615296190	8.9283420219706553	17.2007931177307540	T	T	T
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1.7101779908962633	7.1173640901241653	17.9188236598104602	T	T	T
2.9498121821395262	8.8894734371394932	15.0882839229845729	T	T	T
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3.3877781647846335	7.2368382427109568	19.1415235248587372	T	T	T
4.9145599045014645	8.8069647509679108	18.5885990500993330	T	T	T
9.5016478132096349	1.7774632990520820	7.9999999999999991	F	F	F
12.1632003207601898	0.0000000724240086	8.3161459287561925	F	F	F
8.2221099291517028	0.0000001771746555	8.9009207394719176	F	F	F
7.3915804039980744	1.7774634208273368	9.4856979795260195	F	F	F
10.0531329871708817	0.0000002313825588	9.8018440286466415	F	F	F
11.5026369249808411	1.7774634713412369	10.9713994226004097	F	F	F
7.9430683680047220	0.0000002447131640	11.2875453513566022	F	F	F
10.2230990409229072	0.0000003494638106	11.8723201620723273	F	F	F
11.3326708689773223	1.7774633167543032	8.9009233068204310	F	F	F
9.3925695157692779	1.7774635931164922	12.4570974021264291	F	F	F
12.0541220989420843	0.0000004036717139	12.7732434512470512	F	F	F
7.2374979687515939	1.7834950577194195	13.9885169483943006	T	T	T
9.9053961163922963	0.0265909751223045	14.3107726436215295	T	T	T
12.2339633296672066	-0.0174531764069513	14.8566021215249471	T	T	T
7.1125389162218573	1.7774634890434580	11.8723227294208407	F	F	F
11.3809371864037665	1.7741937107934518	15.5824763015084553	T	T	T
7.7284465603942527	-0.0384686058305428	15.8705281452014013	T	T	T
9.1838708894380936	1.7372056732722718	17.0010145709901259	T	T	T

11.9618987899520519	-0.0693972059687455	17.2717401423483672	T	T	T
7.9954140419176127	-0.0492242775595650	17.9114165198332707	T	T	T
9.0514785256825725	1.7591914654480023	14.9382985986917074	T	T	T
7.2886006217852426	1.7574936857572139	18.8219503853484795	T	T	T
9.9129327882184217	0.0426673730164671	18.8240136155013040	T	T	T
11.1170122332086603	1.7845317209919263	17.8587174167617739	T	T	T
9.5016475194371672	5.3323896216387361	7.9999999999999991	F	F	F
12.1632000269877167	3.5549263950106638	8.3161459287561925	F	F	F
8.2221096353792316	3.5549264997613097	8.9009207394719176	F	F	F
7.3915801102256031	5.3323897434139917	9.4856979795260195	F	F	F
10.0531326933984140	3.5549265539692136	9.8018440286466415	F	F	F
11.5026366312083717	5.3323897939278915	10.9713994226004097	F	F	F
7.9430680742322526	3.5549265672998192	11.2875453513566022	F	F	F
10.2230987471504378	3.5549266720504651	11.8723201620723273	F	F	F
11.3326705752048511	5.3323896393409580	8.9009233068204310	F	F	F
9.3925692219968084	5.3323899157031471	12.4570974021264291	F	F	F
12.0541218051696166	3.5549267262583686	12.7732434512470512	F	F	F
7.2658909331512707	5.3196139139337006	13.9806044016171800	T	T	T
9.8686090569040061	3.5235849815377200	14.3394796808170017	T	T	T
12.1709848997887917	3.5645039359989141	14.8583619077853513	T	T	T
7.1125386224493878	5.3323898116301134	11.8723227294208407	F	F	F
11.2985915016049745	5.3409644578954154	15.3374350385613685	T	T	T
7.6840699531972776	3.5922976392842045	15.9443602517449019	T	T	T
9.3039740474289268	5.3169672340161842	17.1220077839775371	T	T	T
11.9456841697166194	3.6423446223890594	17.2776036565903084	T	T	T
8.0150744047956533	3.5190185606038193	17.9696679951076135	T	T	T
9.0942638221799186	5.3309321323253887	15.0195617638838055	T	T	T
7.2524067110728518	5.2996667464597804	18.7516274708615462	T	T	T
9.9232681236335658	3.3544847736840797	18.8524195699343693	T	T	T
11.1408311476659527	5.3588867507619655	18.2348370834186824	T	T	T
9.5016472256646978	8.8873159442253922	7.9999999999999991	F	F	F
12.1631997332152491	7.1098527175973194	8.3161459287561925	F	F	F
8.2221093416067621	7.1098528223479658	8.9009207394719176	F	F	F
7.3915798164531328	8.8873160660006469	9.4856979795260195	F	F	F
10.0531323996259410	7.1098528765558680	9.8018440286466415	F	F	F
11.5026363374359004	8.8873161165145458	10.9713994226004097	F	F	F
7.9430677804597831	7.1098528898864739	11.2875453513566022	F	F	F
10.2230984533779683	7.1098529946371203	11.8723201620723273	F	F	F
11.3326702814323834	8.8873159619276141	8.9009233068204310	F	F	F
9.3925689282243408	8.8873162382898006	12.4570974021264291	F	F	F
12.0541215113971472	7.1098530488450233	12.7732434512470512	F	F	F
7.2631464380994855	8.8762386348894573	13.9773085665138623	T	T	T
9.8368076904028765	7.1109554743212442	14.3042192219570268	T	T	T
12.1525169255798513	7.1202770153490009	14.8448630257630185	T	T	T
7.1125383286769193	8.8873161342167659	11.8723227294208407	F	F	F
11.3132151804965826	8.8895586403567126	15.3702536502366431	T	T	T
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Oxide reference: ZrO2(101)/fcc(100)_7x4/Ru E_tot= -2072.28822987 eV
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Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr  O Zr
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Selective dynamics
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Metal reference: ZrO2(101)/fcc(100)_7x4/Ru E_tot= -717.39146368 eV
 D3-zero damping= -26.5100811 eV, D3-BJ damping= -32.3342088 eV
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  84
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 13.3342881087874421 -0.0000000000000000  8.0058917535084664
 14.6639552466384000  1.3318783400796339  9.8331867893550466
 13.3334872602096333 -0.0000000000000000 11.6600660691660050
 13.3280741648898573  2.6661947419400005  8.0046169725488046
 14.6639553234911943  4.0005111121559578  9.8331867449763859
 13.3280339139005495  2.6661947419400005 11.6614671175594644
 13.3342881072061559  5.3323894838800010  8.0058917015457016
 14.6639553402302010  6.6642678458438862  9.8331869119866813
 13.3334872602096333  5.3323894379200487 11.6600660691660050
 13.3280742311681788  7.9985842258200019  8.0046169844392310
 14.6639553861901533  9.3329006736403226  9.8331867893550466
 13.3280339784327211  7.9985842258200019 11.6614670331852057
 16.0048934483644310 -0.0000000000000000  7.9999333125018808
 17.3303214158427998  1.3357770685641999  9.8333963088984699
 16.0045066704117431 -0.0000000000000000 11.6662992145843969
 15.9954790922908039  2.6661946396267315  8.0041737909099897
 17.3303213698828529  3.9966122677663076  9.8333963305490464
 15.9953874546844510  2.6661946959800451 11.6631596869220093
 16.0048934026381460  5.3323894838800010  7.9999333240987758
 17.3303214834533428  6.6681665307936004  9.8333960608817854
 16.0045066244517820  5.3323894838800010 11.6662991986726041
 15.9954790136079108  7.9985842258200019  8.0041736885967261
 17.3303213698828529  9.3290017340156162  9.8333960750324927
 15.9953875882643590  7.9985842258200019 11.6631596242199240

Interface: 2O-g-Al2O3(110)/fcc(100)_3x3/Au E_tot= -830.70856315 eV
 D3-zero damping= -36.0904863 eV, D3-BJ damping= -40.359173 eV
 O Al  O Al  O Al  O Au
 1.0000000000000000
     8.6962551314100036    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6962551314100036    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.9340287982870663
  18  12  24  16  12   8   2  45
Selective dynamics
Cartesian
  3.5310462835323402  7.8063656642957868 10.9423958550990683   F   F   F
  7.9821910815116253  5.3364790554512664  9.3854545373318210   F   F   F
  3.5321145935263831  7.4284524359483344  8.0000187449185951   F   F   F
  3.6344616810693871  3.3543474123970207  8.1990827428381010   F   F   F
  7.8802281380900832  1.2624174968523383  9.5845317789161726   F   F   F
  3.6271666011832795  3.1554369468752417 10.8220669229527680   F   F   F
  0.7083960021202884  3.3544316428158409  8.1993257849376384   F   F   F
  5.1588358854150016  1.2623087994643727  9.5846030099037201   F   F   F
  0.7160901952006844  3.1553045949744871 10.8217845066302907   F   F   F
  0.8118413287580194  7.8064783860657743 10.9423584978630899   F   F   F
  5.0560005793416138  5.3365720443687925  9.3853700880230981   F   F   F
  0.8106713855975951  7.4281840563327339  8.0000000000000000   F   F   F
  6.5192511574305740  7.6188020475596341 10.9172067463060003   F   F   F
  6.5192057185729801  7.7314754794541836  8.0327436308783255   F   F   F
  2.1717681959075095  0.9592602948928505  9.5519775531218265   F   F   F
  2.1716499835923124  5.5649932499595769  9.4220834377914784   F   F   F
  6.5193476785207736  3.1257350510745350  8.1626394660302282   F   F   F
  6.5194342443598448  3.2340497157512256 10.8301543211852653   F   F   F
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0.6529590787385497	5.3305977833481926	8.0560139425344559	F	F	F
5.0011162574095147	3.3603749684517115	9.5285274732362595	F	F	F
0.6828365157980596	1.1907892444500303	10.9191009939757393	F	F	F
8.0377282287004821	3.3603184787138018	9.5284873332419124	F	F	F
3.6599190301032727	1.1908533309865517	10.9192047381793635	F	F	F
3.6895912828186770	5.3305164729746144	8.0559839586400095	F	F	F
6.5190859549397233	1.0905682195122306	8.1168144920444938	F	F	F
6.5194715415604199	1.0897006865345162	10.8835529458276739	F	F	F
6.5191569704862573	6.4821600504198278	9.4463612987341463	F	F	F
2.1718420852423406	7.6002031203212406	9.4677862360962415	F	F	F
2.1714813503303882	2.2087144238198260	8.1383270166926529	F	F	F
2.1715979796152878	4.3361109845775054	10.8469192662674665	F	F	F
3.4758751066452569	7.9322576436813232	16.4173113916098075	T	T	T
7.9630646740379083	5.2478650479284497	14.9004337889711209	T	T	T
3.5321145935263831	7.4284524359483344	13.5580397357678457	F	F	F
7.9747256490413179	5.5352448492610788	12.3205669558782276	F	F	F
7.8788760809173155	0.8845355344362547	12.2001224306209899	F	F	F
3.6344616810693871	3.3543474123970207	13.7571037336873516	F	F	F
7.8430200847838840	1.3298472968417856	15.0593023540937896	T	T	T
3.6295118277590297	3.0498191515228208	16.3087106231323737	T	T	T
5.1596266770472559	0.8844520387713608	12.2001609218852352	F	F	F
0.7083960021202884	3.3544316428158409	13.7573467757868890	F	F	F
5.2029328005660878	1.3252945980810276	15.0651835541435020	T	T	T
0.7300687012909104	3.0566931048070463	16.3025188426282526	T	T	T
0.8819535922317694	7.9258024517288943	16.4304957072980748	T	T	T
5.0804330189800044	5.2482256695389049	14.8984553824512584	T	T	T
0.8106713855975951	7.4281840563327339	13.5580209908492506	F	F	F
5.0637449340171754	5.5351531724033096	12.3204488991888077	F	F	F
6.5473943114070545	7.4615343392909503	16.3742784457916279	T	T	T
6.5192057185729801	7.7314754794541836	13.5907646217275762	F	F	F
2.1714213028133433	1.0719992175167494	12.2256103096605884	F	F	F
2.1725253022714632	0.9953278843090991	15.0542812197495444	T	T	T
2.1748806563186092	5.5290808934668352	14.8953737755303042	T	T	T
2.1715094718585832	5.4566459574430537	12.3122395822918378	F	F	F
6.5193476785207736	3.1257350510745350	13.7206604568794788	F	F	F
6.5213154594159324	3.2217286401635241	16.2978139124773556	T	T	T
0.6529590787385497	5.3305977833481926	13.6140349333837065	F	F	F
5.0307943322257458	7.4998334412120302	12.2234202596149437	F	F	F
5.0259243595768597	3.3452378817686550	15.0173844965438299	T	T	T
0.6793803054109018	1.1665668743123687	16.3772071098059442	T	T	T
8.0202309381089893	3.3448682648514385	15.0203853713155961	T	T	T
3.6912585658825150	1.1568360202970724	16.3813699457497606	T	T	T
3.6895912828186770	5.3305164729746144	13.6140049494892601	F	F	F
8.0078230000662902	7.4998959336838711	12.2233730105456431	F	F	F
6.5190859549397233	1.0905682195122306	13.6748354828937444	F	F	F
6.5282883374366252	1.2256709636831529	16.3630770714763685	T	T	T
6.5229699855960455	6.3732699081544597	14.9380056177687415	T	T	T
2.1775617601700552	7.6148000598467309	15.0362584001403530	T	T	T
2.1713481796615515	7.6013207773936822	12.2590327337071869	F	F	F
2.1714813503303882	2.2087144238198260	13.6963480075419035	F	F	F
2.1804911617448459	4.1358018512749943	16.1383786507680149	T	T	T
6.5192328367062737	4.3545065208273153	12.2955930440659955	F	F	F
3.5918014324700529	7.1373340188256122	18.8027767126944880	T	T	T
7.8436915549584905	5.4346123719508466	17.8468311902495778	T	T	T
7.9072484659917475	0.8683879255668556	17.5784268144727243	T	T	T
3.5727123500973605	3.6677797430130270	19.2855087883051262	T	T	T
5.1873424708925562	0.8315241782550497	17.5984325388402674	T	T	T
0.8385823127481679	3.5734182275435629	19.2841624619982639	T	T	T
0.7713234913718509	7.0874516153276801	18.8137959520776477	T	T	T
5.2190955685588794	5.4945591307429416	17.8224690918811923	T	T	T
6.5451385751226665	7.8441564548823388	18.9013727952668447	T	T	T
2.1876437125618335	1.1273099529376380	17.7816676389500117	T	T	T
2.1820307517640920	5.2051494589413636	17.5757176181778227	T	T	T

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  6.4604420672541387  2.9111712682562687 18.9665500172958659   T   T   T
  0.6976124802660578  5.2188636196575482 18.6258263965147890   T   T   T
  5.1540362324098874  7.4663257736564681 17.7319800208888445   T   T   T
  3.6757477495830964  5.2887763455449619 18.6085365794705133   T   T   T
  7.9194854863237785  7.3851471658094701 17.7335792197609230   T   T   T
  6.6585822128232897  1.0630906565572749 18.9678800089960866   T   T   T
  2.1718526604493698  7.8489395407354046 17.8720785668267688   T   T   T
  2.2436109628478151  2.4654002637562735 19.1058515422666702   T   T   T
  6.5023577568804427  4.2461634967475250 17.8205789285438883   T   T   T
  2.4245884939196887  1.5429471692599939 20.5943643581213749   T   T   T
  7.1914214494048903  1.1356822734379868 20.6810560102026102   T   T   T
  0.1542673830315473  0.1671440115535309 21.7462865700796399   T   T   T
  1.6062454776653916  1.7421696930562780 23.7406400179870936   T   T   T
  0.1352194668707822  0.2432456840689146 25.7918485051388124   T   T   T
  0.8518617771871160  3.3664866069087487 21.5897126662970713   T   T   T
  1.7592049284001963  4.6118911891770775 23.8320723620611830   T   T   T
  0.1801432149891467  3.1620227534472543 25.8127128630427940   T   T   T
  0.2988644550643078  6.0846736173479998 21.6242072443787485   T   T   T
  1.5846034783186891  7.5500650859660681 23.7475740047790715   T   T   T
  0.1452073338084851  6.0253509931667528 25.7684306410034552   T   T   T
  2.8976669378549840 -0.3786752623811387 21.3233290186651487   T   T   T
  4.4836439285214542  1.6879947921956022 23.7531166092185835   T   T   T
  3.0393732925079640  0.2582379485591133 25.8005243928701375   T   T   T
  4.0180636740002891  3.0803225492429300 21.4764813195632094   T   T   T
  4.7208238711695030  4.5196693007750479 23.7371813414215396   T   T   T
  3.1191062453056273  3.1458579443848929 25.8290799433388187   T   T   T
  3.2349750740494794  5.7417408723043923 21.6795853339984141   T   T   T
  4.4340616846623764  7.4237183081013418 23.7520624061720831   T   T   T
  3.0791769512182108  6.0588677346517894 25.8191866608691605   T   T   T
  5.6084902024712875  0.0695744389142692 21.7361998905016272   T   T   T
  7.3838921690796129  1.6923824083125147 23.7387307214153509   T   T   T
  5.9262597120023059  0.2224978063207799 25.7765274592278502   T   T   T
  6.7739800193792696  3.4482064778091353 21.1208172605311866   T   T   T
  7.5414114919737223  4.4874077355297741 23.5662375674991793   T   T   T
  6.0271606487588576  3.1273085352720824 25.8276500471316659   T   T   T
  6.1129622083171951  6.0431674122777315 21.5009887374454749   T   T   T
  7.3579114339571907  7.4474487168554377 23.7258824914420856   T   T   T
  5.9899675379769288  6.0075646085991536 25.7787122012957362   T   T   T
  1.6140166478408722  1.6921063935592744 27.8558630159760803   T   T   T
  0.1626701407721311  0.2352556001799050 29.9425399104475538   T   T   T
  1.6355036999712382  4.6036546204616560 27.8567230950746350   T   T   T
  0.1881903378882479  3.1374017793885467 29.9366472842255362   T   T   T
  1.6031652574569752  7.4913096340877336 27.8526703083094596   T   T   T
  0.1812706833301406  6.0462014098789876 29.9411920159926090   T   T   T
  4.5275324050576717  1.6776073240093781 27.8655447957179803   T   T   T
  3.0630038559948631  0.2359997249601382 29.9277790307867733   T   T   T
  4.5408034911570887  4.5907963466621222 27.8630204894182789   T   T   T
  3.0807221711857187  3.1353099337366608 29.9312833172264234   T   T   T
  4.5169079322207102  7.4818887707031179 27.8564211499402568   T   T   T
  3.0745076866864411  6.0390106013145788 29.9346733723388283   T   T   T
  7.4273050618072194  1.6725531761043038 27.8660177410909995   T   T   T
  5.9641217291338089  0.2276989968186066 29.9410543914278975   T   T   T
  7.4351223979496401  4.5975510693011152 27.8805211432655184   T   T   T
  5.9814098499452371  3.1224419736510693 29.9308882404446770   T   T   T
  7.4042139485705594  7.4801568892075743 27.8436356856707867   T   T   T
  5.9723093344387701  6.0400165219649971 29.9424423841155729   T   T   T

Oxide reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Au E_tot= -686.25910453 eV
 D3-zero damping= -9.6528228 eV, D3-BJ damping= -14.7720525 eV
 O Al  O Al  O Al  H  O  H  O  H
 1.0000000000000000
     8.6962551314100036    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6962551314100036    0.0000000000000000
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     0.0000000000000000    0.0000000000000000   28.6840463963622163
  18  12  24  16  12   8   1   1   1   1   2
Selective dynamics
Cartesian
  3.5310462835323402  7.8063656642957868 10.9423958550990683   F   F   F
  7.9821910815116253  5.3364790554512664  9.3854545373318210   F   F   F
  3.5321145935263831  7.4284524359483344  8.0000187449185951   F   F   F
  3.6344616810693871  3.3543474123970207  8.1990827428381010   F   F   F
  7.8802281380900832  1.2624174968523383  9.5845317789161726   F   F   F
  3.6271666011832795  3.1554369468752417 10.8220669229527680   F   F   F
  0.7083960021202884  3.3544316428158409  8.1993257849376384   F   F   F
  5.1588358854150016  1.2623087994643727  9.5846030099037201   F   F   F
  0.7160901952006844  3.1553045949744871 10.8217845066302907   F   F   F
  0.8118413287580194  7.8064783860657743 10.9423584978630899   F   F   F
  5.0560005793416138  5.3365720443687925  9.3853700880230981   F   F   F
  0.8106713855975951  7.4281840563327339  8.0000000000000000   F   F   F
  6.5192511574305740  7.6188020475596341 10.9172067463060003   F   F   F
  6.5192057185729801  7.7314754794541836  8.0327436308783255   F   F   F
  2.1717681959075095  0.9592602948928505  9.5519775531218265   F   F   F
  2.1716499835923124  5.5649932499595769  9.4220834377914784   F   F   F
  6.5193476785207736  3.1257350510745350  8.1626394660302282   F   F   F
  6.5194342443598448  3.2340497157512256 10.8301543211852653   F   F   F
  0.6529590787385497  5.3305977833481926  8.0560139425344559   F   F   F
  5.0011162574095147  3.3603749684517115  9.5285274732362595   F   F   F
  0.6828365157980596  1.1907892444500303 10.9191009939757393   F   F   F
  8.0377282287004821  3.3603184787138018  9.5284873332419124   F   F   F
  3.6599190301032727  1.1908533309865517 10.9192047381793635   F   F   F
  3.6895912828186770  5.3305164729746144  8.0559839586400095   F   F   F
  6.5190859549397233  1.0905682195122306  8.1168144920444938   F   F   F
  6.5194715415604199  1.0897006865345162 10.8835529458276739   F   F   F
  6.5191569704862573  6.4821600504198278  9.4463612987341463   F   F   F
  2.1718420852423406  7.6002031203212406  9.4677862360962415   F   F   F
  2.1714813503303882  2.2087144238198260  8.1383270166926529   F   F   F
  2.1715979796152878  4.3361109845775054 10.8469192662674665   F   F   F
  3.4742794148779859  7.9268818728363835 16.4593929378543748   T   T   T
  7.9609477832512026  5.2648822143914460 14.9031838220319948   T   T   T
  3.5321145935263831  7.4284524359483344 13.5580397357678457   F   F   F
  7.9747256490413179  5.5352448492610788 12.3205669558782276   F   F   F
  7.8788760809173155  0.8845355344362547 12.2001224306209899   F   F   F
  3.6344616810693871  3.3543474123970207 13.7571037336873516   F   F   F
  7.8300465586113690  1.2703259674620271 15.0727933607588049   T   T   T
  3.6230068598565635  3.0482839677855575 16.2940353664207045   T   T   T
  5.1596266770472559  0.8844520387713608 12.2001609218852352   F   F   F
  0.7083960021202884  3.3544316428158409 13.7573467757868890   F   F   F
  5.2079593065244056  1.2756423089970168 15.0446967129485270   T   T   T
  0.6909074646483774  3.0452923556068101 16.3054237815334382   T   T   T
  0.8871390888090505  7.9196448175813998 16.4569931363180260   T   T   T
  5.0687823765975786  5.2678782716058592 14.9031738104854874   T   T   T
  0.8106713855975951  7.4281840563327339 13.5580209908492506   F   F   F
  5.0637449340171754  5.5351531724033096 12.3204488991888077   F   F   F
  6.4875036057686479  7.5243406036596285 16.3704437451938034   T   T   T
  6.5192057185729801  7.7314754794541836 13.5907646217275762   F   F   F
  2.1714213028133433  1.0719992175167494 12.2256103096605884   F   F   F
  2.1714461159557654  0.9930264474984484 15.0659250676279015   T   T   T
  2.1667450797354442  5.5272461470266947 14.9009360023410196   T   T   T
  2.1715094718585832  5.4566459574430537 12.3122395822918378   F   F   F
  6.5193476785207736  3.1257350510745350 13.7206604568794788   F   F   F
  6.5067504506023424  3.3044771492689207 16.2576272855769766   T   T   T
  0.6529590787385497  5.3305977833481926 13.6140349333837065   F   F   F
  5.0307943322257458  7.4998334412120302 12.2234202596149437   F   F   F
  5.0413403696173367  3.3379968660947439 15.0304609643876343   T   T   T
  0.6752429522170678  1.1630666779320711 16.4179122506047364   T   T   T
  7.9888907447241895  3.3339112734050476 15.0290821832436894   T   T   T
```

```
  3.6496791784855791  1.1746790437080079 16.3742701258108490   T   T   T
  3.6895912828186770  5.3305164729746144 13.6140049494892601   F   F   F
  8.0078230000662902  7.4998959336838711 12.2233730105456431   F   F   F
  6.5190859549397233  1.0905682195122306 13.6748354828937444   F   F   F
  6.5144429723324597  0.7994531009838225 16.2685195936423241   T   T   T
  6.5152063349498874  6.3700143930172395 14.9143280982314952   T   T   T
  2.1663082407548724  7.6032299935486565 15.0486003041611340   T   T   T
  2.1713481796615515  7.6013207773936822 12.2590327337071869   F   F   F
  2.1714813503303882  2.2087144238198260 13.6963480075419035   F   F   F
  2.1585701582204671  4.1102254068217814 16.1206176495704341   T   T   T
  6.5192328367062737  4.3545065208273153 12.2955930440659955   F   F   F
  3.5682831445308634  7.0475363497052461 18.8416164452887180   T   T   T
  7.8440600060308991  5.5170907053314080 17.8502264646524225   T   T   T
  7.8579080974358595  0.7694268404930591 17.6071800449869649   T   T   T
  3.5869558984381631  3.6267504351755266 19.3971306364087468   T   T   T
  5.1430215252160547  0.8785998289787230 17.5340806834686340   T   T   T
  0.7557038808457852  3.6221618033169807 19.3555101401779908   T   T   T
  0.7864316885310446  7.0894323039181328 18.8773849312402326   T   T   T
  5.2285197561761185  5.4498669415962464 17.8523672700159146   T   T   T
  6.4654332603988331  7.9128427198151359 18.9570306755432121   T   T   T
  2.1425870789630306  1.1486864068288458 17.8122881656877148   T   T   T
  2.1793753728650191  5.1501960294799094 17.5780600895252022   T   T   T
  6.8982886484168349  2.9296278088523873 18.9589161630268066   T   T   T
  0.7068522325391597  5.2328966186822274 18.6113737424940027   T   T   T
  5.0817218759557576  7.3830021663204706 17.7812180933000015   T   T   T
  3.6656900850069376  5.1907554893854337 18.6107082198143345   T   T   T
  7.9362245391949040  7.4630593856083678 17.8425446465054307   T   T   T
  6.3516354155326056  1.0805402749911088 18.8855251838208709   T   T   T
  2.1764109746733213  7.8561622210441913 17.9146478675362850   T   T   T
  2.1773105939745436  2.5213696071075784 19.2819660345183514   T   T   T
  6.5676188982637784  4.2833446036074445 17.7294566890272733   T   T   T
  7.8834658403195492  3.0779830368493553 19.2197853693996166   T   T   T
  2.5093337321311036  1.3470231856917345 20.5624395281847860   T   T   T
  1.9503509997582893  0.5728628133438490 20.7275263499375555   T   T   T
  5.1468108582960905  1.5576101953260357 20.2615828776418994   T   T   T
  4.7895034738179243  2.4913734962467768 20.0608920748519814   T   T   T
  4.2758450807188835  1.0875741728940489 20.4630729281785442   T   T   T

Metal reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Au E_tot= -159.69647968 eV
 D3-zero damping= -22.8620021 eV, D3-BJ damping= -22.7531399 eV
Au
 1.0000000000000000
     8.6962551314100036    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6962551314100036    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0004513041461060 -0.0004521478249009  7.6902785096333410
  1.4488052971537153  1.4488046968689963  9.7642512387830838
 -0.0003264515018972 -0.0003264029968842 11.8274829358139009
  1.4486340926622530  1.4486343530167267 13.8909255075381193
 -0.0004930902193350 -0.0004923822173292 15.9656612773392474
 -0.0004513617372237  2.8982995115579913  7.6902784933907125
  1.4488053392557636  4.3475563251389504  9.7642512352211579
 -0.0003264279439596  2.8984253026937727 11.8274829059435724
  1.4486340295025690  4.3473860924052010 13.8909254347227034
 -0.0004930904740366  2.8982594410924225 15.9656613404989258
 -0.0004512985775402  5.7970511990889966  7.6902784933907169
  1.4488051905304458  7.2463081367532558  9.7642511955601989
 -0.0003264517565989  5.7971770179431026 11.8274828729790009
  1.4486341579076387  7.2461378028752028 13.8909253911364345
 -0.0004931029000373  5.7970111515624252 15.9656613056681724
  2.8983003716717768 -0.0004522366947585  7.6902784933907125
```

```
  4.3475570286456895  1.4488047260715566  9.7642511678716559
  2.8984253092507504 -0.0003264029968842 11.8274828335121409
  4.3473858347452996  1.4486343530167267 13.8909254190744971
  2.8982586970342292 -0.0004922693775838 15.9656612935818725
  2.8983003720291745  2.8982994886189934  7.6902785070146065
  4.3475570286456895  4.3475563970806954  9.7642511736949427
  2.8984253092507504  2.8984252443134291 11.8274828892216242
  4.3473857400521627  4.3473860924052010 13.8909253687918497
  2.8982586467515858  2.8982594675933426 15.9656614191104769
  2.8983003557865490  5.7970511990889966  7.6902785482205562
  4.3475569832005041  7.2463081367532558  9.7642510417941732
  2.8984252201261906  5.7971770682257473 11.8274828112504462
  4.3473857402973612  7.2461377478132150 13.8909253687918497
  2.8982586364932907  5.7970111515624252 15.9656613955609075
  5.7970521511573496 -0.0004521751685466  7.6902784933907125
  7.2463087391156904  1.4488046968689963  9.7642512352211579
  5.7971769166651548 -0.0003264029968842 11.8274828226963553
  7.2461374633196218  1.4486343819351910 13.8909254347227034
  5.7970103342825920 -0.0004924473054639 15.9656612935818725
  5.7970521771922900  2.8982995115579913  7.6902784933907125
  7.2463087731557092  4.3475564365415504  9.7642512122821632
  5.7971769811335330  2.8984252782705524 11.8274828744101548
  7.2461374004847201  4.3473860634867476 13.8909253844400613
  5.7970103077816715  2.8982593263242200 15.9656613276218913
  5.7970521223624498  5.7970511990889966  7.6902784766687624
  7.2463086840537079  7.2463080967289084  9.7642511933378948
  5.7971769182986375  5.7971770682257473 11.8274827578860258
  7.2461374001599355  7.2461378028752010 13.8909253681974363
  5.7970102801833221  5.7970109736345403 15.9656613029665326

Interface: 2O-g-Al2O3(110)/fcc(100)_3x3/Ag E_tot= -805.81908825 eV
 D3-zero damping= -30.0776215 eV, D3-BJ damping= -38.5443729 eV
 O Al  O Al  O Al  O Ag
 1.0000000000000000
     8.6415811558500017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6415811558500017    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.2716937760818396
  18  12  24  16  12   8   2  45
Selective dynamics
Cartesian
  3.5088463439848243  7.7572864872140848 10.9423958550990683   F   F   F
  7.9320064775055261  5.3029282314419337  9.3854545373318210   F   F   F
  3.5099079374378253  7.3817492262569910  8.0000187449185951   F   F   F
  3.6116115615499145  3.3332583912409213  8.1990827428381010   F   F   F
  7.8306845823734390  1.2544805881109971  9.5845317789161726   F   F   F
  3.6043623463507752  3.1355984899868905 10.8220669229527680   F   F   F
  0.7039422659865778  3.3333420920970971  8.1993257849376384   F   F   F
  5.1264019166715498  1.2543725741112535  9.5846030099037201   F   F   F
  0.7115880851269187  3.1354669701919655 10.8217845066302907   F   F   F
  0.8067372244859640  7.7573985002942738 10.9423584978630899   F   F   F
  5.0242131434937596  5.3030206357315102  9.3853700880230981   F   F   F
  0.8055746368415397  7.3814825339631538  8.0000000000000000   F   F   F
  6.4782641609516567  7.5709020962989797 10.9172067463060003   F   F   F
  6.4782190077713988  7.6828671422999957  8.0327436308783255   F   F   F
  2.1581141345361776  0.9532293570781101  9.5519775531218265   F   F   F
  2.1579966654302276  5.5300057409292931  9.4220834377914784   F   F   F
  6.4783600752068864  3.1060833321211403  8.1626394660302282   F   F   F
  6.4784460968003605  3.2137170147843279 10.8301543211852653   F   F   F
  0.6488538784916427  5.2970839353155723  8.0560139425344559   F   F   F
  4.9696738832037806  3.3392480516212739  9.5285274732362595   F   F   F
  0.6785434739757958  1.1833026676345666 10.9191009939757393   F   F   F
  7.9871944586933639  3.3391919170383710  9.5284873332419124   F   F   F
  3.6369088584167617  1.1833663512544670 10.9192047381793635   F   F   F
```

3.6663945595653988	5.2970031361461061	8.0559839586400095	F	F	F
6.4780999971006361	1.0837117394206146	8.1168144920444938	F	F	F
6.4784831595107777	1.0828496606845370	10.8835529458276739	F	F	F
6.4781705661673703	6.4414062483731760	9.4463612987341463	F	F	F
2.1581875593234963	7.5524201018411805	9.4677862360962415	F	F	F
2.1578290923776358	2.1948280788814425	8.1383270166926529	F	F	F
2.1579449884059114	4.3088495458991538	10.8469192662674665	F	F	F
3.4449140131969092	7.8537388321330228	16.4714598759699911	T	T	T
7.9152238272434525	5.2372780598629891	14.9082696044100373	T	T	T
3.5099079374378253	7.3817492262569910	13.5580397357678457	F	F	F
7.9245879807410207	5.5004443705453570	12.3205669558782276	F	F	F
7.8293410256804412	0.8789743965141341	12.2001224306209899	F	F	F
3.6116115615499145	3.3332583912409213	13.7571037336873516	F	F	F
7.7880619756207148	1.2767130230910269	15.0628122715926942	T	T	T
3.6044729931485158	3.0442082736388536	16.3192255876881127	T	T	T
5.1271877365404732	0.8788914257924338	12.2001609218852352	F	F	F
0.7039422659865778	3.3333420920970971	13.7573467757868890	F	F	F
5.1543844539776140	1.2793184821358610	15.0627938045819381	T	T	T
0.7074165011594036	3.0364543274542330	16.3065286875124649	T	T	T
0.8658179321419223	7.8470629850262368	16.4459656157149254	T	T	T
5.0417767198482659	5.2341302332775452	14.9082684040165816	T	T	T
0.8055746368415397	7.3814825339631538	13.5580209908492506	F	F	F
5.0319088088597432	5.5003532700665243	12.3204488991888077	F	F	F
6.4742786741582563	7.5084657261256451	16.3632898646627858	T	T	T
6.4782190077713988	7.6828671422999957	13.5907646217275762	F	F	F
2.1577694223836081	1.0652594820635937	12.2256103096605884	F	F	F
2.1595885742115177	0.9741031459848163	15.0591578377288826	T	T	T
2.1601139140847030	5.5015051347599488	14.8945386911036106	T	T	T
2.1578570371037791	5.4223396355598270	12.3122395822918378	F	F	F
6.4783600752068864	3.1060833321211403	13.7206604568794788	F	F	F
6.4729580743966784	3.2232316594058688	16.2845560591161025	T	T	T
0.6488538784916427	5.2970839353155723	13.6140349333837065	F	F	F
4.9991653698492824	7.4526814540551847	12.2234202596149437	F	F	F
5.0075604233761997	3.3190360307542170	15.0385320241924987	T	T	T
0.6685999315106960	1.1489493363565724	16.3601871518334363	T	T	T
7.9415948101078149	3.3253737439584001	15.0420701231162024	T	T	T
3.6505014982048913	1.1611928724447635	16.4080872839377783	T	T	T
3.6663945595653988	5.2970031361461061	13.6140049494892601	F	F	F
7.9574772463621377	7.4527435536324029	12.2233730105456431	F	F	F
6.4780999971006361	1.0837117394206146	13.6748354828937444	F	F	F
6.4628017484433338	0.9465356259635447	16.3229517026058417	T	T	T
6.4764752737051019	6.3495728881908038	14.9384976776305116	T	T	T
2.1619890170889229	7.5473468471697700	15.0455136168435235	T	T	T
2.1576967589622811	7.5535307321239822	12.2590327337071869	F	F	F
2.1578290923776358	2.1948280788814425	13.6963480075419035	F	F	F
2.1539383351240931	4.1106522187523753	16.1225439541882167	T	T	T
6.4782459554110563	4.3271294281020038	12.2955930440659955	F	F	F
3.5067246523451856	7.0772244533355497	18.8983254870792408	T	T	T
7.7313172390645857	5.4429525127680796	17.8201469009230209	T	T	T
7.8580419304209741	0.8137488630415346	17.5740798321967233	T	T	T
3.4234949566199213	3.6525764295406109	19.4034540125679591	T	T	T
5.1202463633855730	0.8069406152733098	17.6101122691962786	T	T	T
0.7258642392656210	3.6067225155693090	19.3286915131246779	T	T	T
0.7219915756623103	7.0526947909892304	18.8665205403335499	T	T	T
5.1349202364216326	5.4694506671969467	17.8387683462846489	T	T	T
6.4503686971204122	7.8044542874375269	18.9416502743251307	T	T	T
2.1443632215079749	1.1352656647444046	17.7591544175620371	T	T	T
2.1284727378911410	5.1877103703814900	17.5573803155166743	T	T	T
6.3400260208692316	2.9187132935621301	18.9993687848785413	T	T	T
0.6378938635883683	5.1827419168230318	18.5791037709159106	T	T	T
5.0410907949195947	7.4346984277829824	17.7823849616075691	T	T	T
3.5968371559564809	5.2095122708309889	18.6128897656625760	T	T	T
7.8395804472654511	7.3715218634058255	17.7653823680650689	T	T	T

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  6.6701935631538420  1.1405075091240826 18.9627569434598264   T   T   T
  2.1249088642104228  7.8086381961311755 17.9007445332231860   T   T   T
  2.0922863010538229  2.4528566431691234 19.1378895856885585   T   T   T
  6.4168226470243805  4.2007874688163689 17.8127047976829047   T   T   T
  2.0548980515824984  1.3052628423748529 20.4762592099682408   T   T   T
  7.4880509520661667  1.0962018890373764 20.5542210723482945   T   T   T
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  1.8430426347707007  1.2111370362772256 23.5582381499316220   T   T   T
  0.4189582615616335 -0.2126236676928512 25.6129853925849780   T   T   T
  0.3501171332279403  2.7106876033995797 21.5418168685248155   T   T   T
  1.8503603751958611  4.0858854225738712 23.6037529755967554   T   T   T
  0.4145995547500712  2.6722854769588045 25.6185720660511826   T   T   T
  0.4224037309753321  5.5040847904627652 21.5926598930410414   T   T   T
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  0.4154629320112145  5.5609709846049160 25.6224936751702650   T   T   T
  3.3254192823407474 -0.3393217865648171 21.3638677553855842   T   T   T
  4.7647882609589018  1.2245031670290476 23.5639162086041978   T   T   T
  3.2933907575171513 -0.2071204532895501 25.6138856862156601   T   T   T
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  4.7938951164250536  4.1251672931180074 23.5859650401466219   T   T   T
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  4.7216157960443086  7.0079427240804426 23.5542391492569507   T   T   T
  3.2953972048908433  5.5647384922418128 25.6015981463838003   T   T   T
  6.0906250050665411 -0.2904422012949907 21.5484378282927267   T   T   T
  7.6251974118100048  1.2352333797800774 23.5710770826104969   T   T   T
  6.1812220061392633 -0.2077894460289780 25.6138261755093950   T   T   T
  6.1775483594477185  2.9382118686749430 21.3204651586610829   T   T   T
  7.5999408821532191  4.1013453553897987 23.5712932605200081   T   T   T
  6.1828848515490247  2.6697682082595606 25.6355478723215420   T   T   T
  6.1833759291842201  5.6392599962879579 21.4496840229727646   T   T   T
  7.6322799985609784  7.0127268182170761 23.5498373823693008   T   T   T
  6.1879483823873569  5.5695216482672842 25.6191665563909794   T   T   T
  1.8556260784226006  1.2364441727641320 27.6668286411483315   T   T   T
  0.4195382271261341 -0.2071494478208147 29.7320069895151455   T   T   T
  1.8655326881399870  4.1165530937928487 27.6524418675192329   T   T   T
  0.4222343104754201  2.6820454802610953 29.7205773164059401   T   T   T
  1.8604535903970170  6.9986837408230382 27.6651873209164307   T   T   T
  0.4222950829759216  5.5561415583558471 29.7128387260179210   T   T   T
  4.7405457196668088  1.2328092275750850 27.6681038357515661   T   T   T
  3.3007738291051756 -0.2032365800963445 29.7187530805060973   T   T   T
  4.7391768654560833  4.1228784485219254 27.6550247801826004   T   T   T
  3.3025101109125936  2.6807359716946046 29.7146249530017101   T   T   T
  4.7402442296198446  7.0020047982155980 27.6586635160417877   T   T   T
  3.3025523704757469  5.5583300475331114 29.7107222051046733   T   T   T
  7.6273132721853703  1.2329788046031622 27.6734991858507122   T   T   T
  6.1791617236071890 -0.2010882684231687 29.7287582422746794   T   T   T
  7.6215489623367079  4.1190451677991309 27.6642212474308273   T   T   T
  6.1802007771509686  2.6813700074693156 29.7155588480415673   T   T   T
  7.6200054502748680  7.0020366621917178 27.6716821097707104   T   T   T
  6.1779409261111935  5.5612768099073771 29.7136944913671250   T   T   T

Oxide reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Ag E_tot= -687.90918753 eV
 D3-zero damping= -9.7921245 eV, D3-BJ damping= -14.9492117 eV
 O Al  O Al  O Al  H  O  H  O  H
 1.0000000000000000
     8.6415811558500017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6415811558500017    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6840463963622163
  18  12  24  16  12   8   1   1   1   1   2
Selective dynamics
Cartesian
  3.5088463439848243  7.7572864872140848 10.9423958550990683   F   F   F
```

7.9320064775055261	5.3029282314419337	9.3854545373318210	F	F	F
3.5099079374378253	7.3817492262569910	8.0000187449185951	F	F	F
3.6116115615499145	3.3332583912409213	8.1990827428381010	F	F	F
7.8306845823734390	1.2544805881109971	9.5845317789161726	F	F	F
3.6043623463507752	3.1355984899868905	10.8220669229527680	F	F	F
0.7039422659865778	3.3333420920970971	8.1993257849376384	F	F	F
5.1264019166715498	1.2543725741112535	9.5846030099037201	F	F	F
0.7115880851269187	3.1354669701919655	10.8217845066302907	F	F	F
0.8067372244859640	7.7573985002942738	10.9423584978630899	F	F	F
5.0242131434937596	5.3030206357315102	9.3853700880230981	F	F	F
0.8055746368415397	7.3814825339631538	8.0000000000000000	F	F	F
6.4782641609516567	7.5709020962989797	10.9172067463060003	F	F	F
6.4782190077713988	7.6828671422999957	8.0327436308783255	F	F	F
2.1581141345361776	0.9532293570781101	9.5519775531218265	F	F	F
2.1579966654302276	5.5300057409292931	9.4220834377914784	F	F	F
6.4783600752068864	3.1060833321211403	8.1626394660302282	F	F	F
6.4784460968003605	3.2137170147843279	10.8301543211852653	F	F	F
0.6488538784916427	5.2970839353155723	8.0560139425344559	F	F	F
4.9696738832037806	3.3392480516212739	9.5285274732362595	F	F	F
0.6785434739757958	1.1833026676345666	10.9191009939757393	F	F	F
7.9871944586933639	3.3391919170383710	9.5284873332419124	F	F	F
3.6369088584167617	1.1833663512544670	10.9192047381793635	F	F	F
3.6663945595653988	5.2970031361461061	8.0559839586400095	F	F	F
6.4780999971006361	1.0837117394206146	8.1168144920444938	F	F	F
6.4784831595107777	1.0828496606845370	10.8835529458276739	F	F	F
6.4781705661673703	6.4414062483731760	9.4463612987341463	F	F	F
2.1581875593234963	7.5524201018411805	9.4677862360962415	F	F	F
2.1578290923776358	2.1948280788814425	8.1383270166926529	F	F	F
2.1579449884059114	4.3088495458991538	10.8469192662674665	F	F	F
3.4593884346029444	7.8697768845118903	16.4727355592891698	T	T	T
7.9114209676630249	5.2348477407802934	14.9089702518936527	T	T	T
3.5099079374378253	7.3817492262569910	13.5580397357678457	F	F	F
7.9245879807410207	5.5004443705453570	12.3205669558782276	F	F	F
7.8293410256804412	0.8789743965141341	12.2001224306209899	F	F	F
3.6116115615499145	3.3332583912409213	13.7571037336873516	F	F	F
7.7917433422613538	1.2632220332355644	15.0704870931474311	T	T	T
3.6013844842898961	3.0385984271728650	16.3002080659147026	T	T	T
5.1271877365404732	0.8788914257924338	12.2001609218852352	F	F	F
0.7039422659865778	3.3333420920970971	13.7573467757868890	F	F	F
5.1660652807790823	1.2683410034340972	15.0469392868042231	T	T	T
0.6881778066760640	3.0357274795949980	16.3121962666605640	T	T	T
0.8764879642260065	7.8617146054447158	16.4721783386252412	T	T	T
5.0374999743861082	5.2378427069846412	14.9094267323988259	T	T	T
0.8055746368415397	7.3814825339631538	13.5580209908492506	F	F	F
5.0319088088597432	5.5003532700665243	12.3204488991888077	F	F	F
6.4510065235576288	7.4929199879180191	16.3764085216573072	T	T	T
6.4782190077713988	7.6828671422999957	13.5907646217275762	F	F	F
2.1577694223836081	1.0652594820635937	12.2256103096605884	F	F	F
2.1572666766144999	0.9818215725038677	15.0722216037291226	T	T	T
2.1540178265908132	5.5000947309164063	14.9087598153730205	T	T	T
2.1578570371037791	5.4223396355598270	12.3122395822918378	F	F	F
6.4783600752068864	3.1060833321211403	13.7206604568794788	F	F	F
6.4685672204442852	3.2493514215826265	16.2682338163235052	T	T	T
0.6488538784916427	5.2970839353155723	13.6140349333837065	F	F	F
4.9991653698492824	7.4526814540551847	12.2234202596149437	F	F	F
5.0059856620193441	3.3157307795643840	15.0310652929016779	T	T	T
0.6728799414670830	1.1599691424851812	16.4251400344972076	T	T	T
7.9444019921858002	3.3115260708231906	15.0288270971996827	T	T	T
3.6278817586431500	1.1709422135319600	16.3854475625405875	T	T	T
3.6663945595653988	5.2970031361461061	13.6140049494892601	F	F	F
7.9574772463621377	7.4527435536324029	12.2233730105456431	F	F	F
6.4780999971006361	1.0837117394206146	13.6748354828937444	F	F	F
6.4758911111349642	0.8472936929473668	16.2831987844049593	T	T	T

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  6.4747587863076284  6.3445342558747138 14.9245989156533216   T   T   T
  2.1542889852138645  7.5537620803499834 15.0544457618912535   T   T   T
  2.1576967589622811  7.5535307321239822 12.2590327337071869   F   F   F
  2.1578290923776358  2.1948280788814425 13.6963480075419035   F   F   F
  2.1461821322605505  4.1014463184516101 16.1376627070890315   T   T   T
  6.4782459554110563  4.3271294281020038 12.2955930440659955   F   F   F
  3.5579101280428440  7.0117972965597559 18.8659704222070879   T   T   T
  7.8023171737144041  5.4795095070185784 17.8409099723335771   T   T   T
  7.8165033638290362  0.7852230039188128 17.6151587177591864   T   T   T
  3.5696220750808028  3.5968346421127673 19.4217197341193142   T   T   T
  5.1082931588073670  0.8917685213381116 17.5497089858690174   T   T   T
  0.7437038751232032  3.5959093283681383 19.3816556522250885   T   T   T
  0.7783588386234356  7.0552105378691286 18.9020566361188003   T   T   T
  5.1954994752921833  5.4106905031099091 17.8453752537589168   T   T   T
  6.4333709967093338  7.8603675643253066 18.9616764880201281   T   T   T
  2.1335358197488712  1.1437606273286156 17.8222227056076044   T   T   T
  2.1678014207794987  5.1291297827175493 17.5992003434764186   T   T   T
  6.8531631962022903  2.9171617242262835 18.9809176360214842   T   T   T
  0.6996112061913350  5.2047738351860051 18.6369163374043332   T   T   T
  5.0537377328902524  7.3415641508354499 17.7789789796426518   T   T   T
  3.6503211974141165  5.1592096122816011 18.6351250819097771   T   T   T
  7.8945102269758154  7.4242365918209270 17.8317950811250725   T   T   T
  6.3147610869252109  1.0735053899559928 18.9055559647653801   T   T   T
  2.1670566150835673  7.8040747161154629 17.9315779729533169   T   T   T
  2.1614088829282241  2.4907729083841184 19.3012243062702993   T   T   T
  6.5303388113641372  4.2455343544098545 17.7328070629710979   T   T   T
  7.8405883132982428  3.0687309236969540 19.2454465468838727   T   T   T
  2.4797738210689673  1.3104626146185734 20.5779893714957183   T   T   T
  1.9246830854456265  0.5307312978267738 20.7300303483978681   T   T   T
  5.1160387563677912  1.5350677188624220 20.2886141202422365   T   T   T
  4.7547510771704866  2.4685538830507174 20.0888927681146114   T   T   T
  4.2483678213460028  1.0589663027825105 20.4877922907717469   T   T   T

Metal reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Ag E_tot= -131.36629926 eV
 D3-zero damping= -16.936569 eV, D3-BJ damping= -20.6475888 eV
Ag
 1.0000000000000000
     8.6415811558500017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6415811558500017    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0001009703296095 -0.0001016700434123  7.7258836695138298
  1.4400307318692709  1.4400300732652214  9.7725647429041853
 -0.0003232964402609 -0.0003231635632294 11.8271512840411095
  1.4394458355100475  1.4394462067322227 13.8829579852519114
 -0.0010923489894180 -0.0010917178330178 15.9300414833092656
 -0.0001009941403956  2.8804254430159308  7.7258837052662743
  1.4400307132981172  4.3205571804376470  9.7725647886942788
 -0.0003232964402608  2.8802039086243814 11.8271512466221989
  1.4394458915001056  4.3199732401110573 13.8829578839549619
 -0.0010923811686901  2.8794353189071793 15.9300413867565762
 -0.0001009703296095  5.7609524949659372  7.7258836084044784
  1.4400307132981172  7.2010841822845135  9.7725649643636974
 -0.0003232594403030  5.7607309641475517 11.8271512840411095
  1.4394458355100475  7.2005002697604734 13.8829580412419666
 -0.0010923811686901  5.7599623708571830 15.9300412646431759
  2.8804260578096073 -0.0001016089340708  7.7258835957202558
  4.3205577100257004  1.4400300732652214  9.7725647565123026
  2.8802038114997974 -0.0003231806241809 11.8271513448518544
  4.3199728374772501  1.4394461507421645 13.8829579852519114
  2.8794346469705299 -0.0010917330428272 15.9300415014219006
  2.8804260578096073  2.8804254430159308  7.7258835928174348
```

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  4.3205577100257004  4.3205571804376470  9.7725647886942788
  2.8802038163204817  2.8802038900532287 11.8271512280510471
  4.3199728136664639  4.3199732401110573 13.8829579852519114
  2.8794347029605878  2.8794353189071793 15.9300415574119558
  2.8804260578096073  5.7609524949659372  7.7258835754826460
  4.3205577100257004  7.2010842382745714  9.7725647370172517
  2.8802038114997974  5.7607309232758146 11.8271512466221989
  4.3199728696565227  7.2005002697604734 13.8829580412419666
  2.8794346843894352  5.7599623708571830 15.9300415400418842
  5.7609531001432535 -0.0001016700434112  7.7258835928174348
  7.2010847993946063  1.4400300732652214  9.7725647886942788
  5.7607308393298959 -0.0003231635632294 11.8271513448518544
  7.2004998894272498  1.4394461098704272 13.8829580181737349
  5.7599616616219746 -0.0010917178330179 15.9300414256492964
  5.7609531224438379  2.8804254430159308  7.7258835531820598
  7.2010847993946063  4.3205571990087996  9.7725649260175373
  5.7607308393298959  2.8802038475150402 11.8271512280510471
  7.2004998656164636  4.3199732348714246 13.8829579852519114
  5.7599617176120343  2.8794353189071793 15.9300413203241078
  5.7609531426814442  5.7609524949659372  7.7258836142914085
  7.2010847619757010  7.2010841822845135  9.7725647429041853
  5.7607307665880105  5.7607309232758146 11.8271512840411095
  7.2004998894272498  7.2005002697604734 13.8829580460626527
  5.7599616616219746  5.7599623708571830 15.9300415014219006

Interface: 2O-g-Al2O3(110)/fcc(100)_3x3/Cu E_tot= -840.04082655 eV
 D3-zero damping= -32.3349713 eV, D3-BJ damping= -42.2095539 eV
 O Al  O Al  O Al  O Cu
 1.0000000000000000
     7.5713089101900026    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.5713089101900026    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.1819614305421808
  18  12  24  16  12   8   2  45
Selective dynamics
Cartesian
  3.0742706814383642  6.7965354071552930 10.9423958550990683   F   F   F
  6.9496160755450562  4.6461529487152262  9.3854545373318210   F   F   F
  3.0752007950165097  6.4675089756823914  8.0000187449185951   F   F   F
  3.1643082791158981  2.9204295489932952  8.1990827428381010   F   F   F
  6.8608430427428830  1.0991113643589845  9.5845317789161726   F   F   F
  3.1579568896376000  2.7472501105824416 10.8220669229527680   F   F   F
  0.6167580046523641  2.9205028833781403  8.1993257849376384   F   F   F
  4.4914896717292514  1.0990167280483447  9.5846030099037201   F   F   F
  0.6234568781037551  2.7471348797031352 10.8217845066302907   F   F   F
  0.7068216598067383  6.7966335472545181 10.9423584978630899   F   F   F
  4.4019571249731957  4.6462339086007374  9.3853700880230981   F   F   F
  0.7058030603129238  6.4672753136124310  8.0000000000000000   F   F   F
  5.6759218341858286  6.6332349909229507 10.9172067463060003   F   F   F
  5.6758822732918386  6.7313330050628108  8.0327436308783255   F   F   F
  1.8908285973753074  0.8351705312417778  9.5519775531218265   F   F   F
  1.8907256769869536  4.8451065823013115  9.4220834377914784   F   F   F
  5.6760058693227018  2.7213904474369603  8.1626394660302282   F   F   F
  5.6760812370181952  2.8156935438133313 10.8301543211852653   F   F   F
  0.5684923931206077  4.6410324770634208  8.0560139425344559   F   F   F
  4.3541726304528670  2.9256773813273207  9.5285274732362595   F   F   F
  0.5945048895347544  1.0367489316290468 10.9191009939757393   F   F   F
  6.9979689459477150  2.9256281990931861  9.5284873332419124   F   F   F
  3.1864724694090163  1.0368047279410977 10.9192047381793635   F   F   F
  3.2123063240941336  4.6409616849872153  8.0559839586400095   F   F   F
  5.6757780022636899  0.9494924830044873  8.1168144920444938   F   F   F
  5.6761137094586616  0.9487371739588352 10.8835529458276739   F   F   F
  5.6758398312500882  5.6436288270516490  9.4463612987341463   F   F   F
  1.8908929283971920  6.6170420180407037  9.4677862360962415   F   F   F
```

1.8905788580977576	1.9229954669488631	8.1383270166926529	F	F	F
1.8906804002363682	3.7751923370469673	10.8469192662674665	F	F	F
3.0744103406371788	6.7532656493438123	16.7411418376118881	T	T	T
6.9998438941957879	4.6927979067356933	15.0337033006386225	T	T	T
3.0752007950165097	6.4675089756823914	13.5580397357678457	F	F	F
6.9431163702665497	4.8192064301244377	12.3205669558782276	F	F	F
6.8596658874772460	0.7701121542613976	12.2001224306209899	F	F	F
3.1643082791158981	2.9204295489932952	13.7571037336873516	F	F	F
6.9271856189453889	1.0013019056923200	15.1981524919528859	T	T	T
3.1908000653902699	2.7850760028211141	16.5177740305815632	T	T	T
4.4921781666780438	0.7700394595828238	12.2001609218852352	F	F	F
0.6167580046523641	2.9205028833781403	13.7573467757868890	F	F	F
4.4322257955109201	1.0034868393825533	15.1945864693934709	T	T	T
0.5980523843191637	2.7865301272237777	16.5203751597810822	T	T	T
0.7000511644568156	6.7171825066183084	16.8100044194085392	T	T	T
4.3695711766889920	4.6934905289196971	14.9995155825017523	T	T	T
0.7058030603129238	6.4672753136124310	13.5580209908492506	F	F	F
4.4086996711235455	4.8191266125708356	12.3204488991888077	F	F	F
5.7306661251908322	6.6336576069361239	16.6683347792582168	T	T	T
5.6758822732918386	6.7313330050628108	13.5907646217275762	F	F	F
1.8905265783182470	0.9333255642403494	12.2256103096605884	F	F	F
1.8810672150273005	0.8525186090587400	15.2374912405967340	T	T	T
1.8943679060019347	4.8379961128820375	15.0264119044623357	T	T	T
1.8906033418294066	4.7507750788174317	12.3122395822918378	F	F	F
5.6760058693227018	2.7213904474369603	13.7206604568794788	F	F	F
5.6843357047341252	2.7848156747183945	16.4060666800285979	T	T	T
0.5684923931206077	4.6410324770634208	13.6140349333837065	F	F	F
4.3800115540927473	6.5296561451253972	12.2234202596149437	F	F	F
4.3359843411824812	2.9167283789742604	15.1384123572044107	T	T	T
0.6081403274951501	1.0199723491889190	16.6716977096259278	T	T	T
7.0272483560536783	2.9107555744460498	15.1434909487297880	T	T	T
3.1604178175023403	1.0328186326521900	16.6631648363810712	T	T	T
3.2123063240941336	4.6409616849872153	13.6140049494892601	F	F	F
6.9719322530726959	6.5297105535807285	12.2233730105456431	F	F	F
5.6757780022636899	0.9494924830044873	13.6748354828937444	F	F	F
5.6785435303359142	0.8995962544583133	16.5280730809296728	T	T	T
5.6815089458544188	5.7738934224700227	15.1265017185751116	T	T	T
1.9088039673874255	6.6176532449808816	15.1594840040556527	T	T	T
1.8904629143660816	6.6180150951668049	12.2590327337071869	F	F	F
1.8905788580977576	1.9229954669488631	13.6963480075419035	F	F	F
1.8934253389340059	3.9042277517520776	16.5217500628127176	T	T	T
5.6759058834275962	3.7912082295675131	12.2955930440659955	F	F	F
3.2652417426822589	6.1849734205427458	19.4641562133783061	T	T	T
6.9479674098392454	4.6753365060708711	18.2318020122200508	T	T	T
6.8798183013428451	0.9337513631624480	17.9389120982076555	T	T	T
2.2231733544757351	3.4768386257491586	20.2050954486081658	T	T	T
4.4483678424080857	0.8576052203575946	17.9170971927516121	T	T	T
-0.0519409966218956	2.6106231448132826	19.8336307486283587	T	T	T
0.6611273578281877	6.2735757298508608	19.5157005295646009	T	T	T
4.3925852693623604	4.8111298138047687	17.7842169704282078	T	T	T
5.7051967025159218	6.8824223135851232	19.3605719604461761	T	T	T
1.8842012380609288	0.9804042508116455	18.1321266772338596	T	T	T
1.9043273329385622	4.6112289411215768	18.1031944640606639	T	T	T
4.8220012366809994	2.9403832238472707	19.3438359027802953	T	T	T
0.6109970257986760	4.3343116431908415	19.4491100608160465	T	T	T
4.4396915735637101	6.5504549945231982	18.0582005746114618	T	T	T
3.4655553250818909	4.2900531490292471	19.1978378133349672	T	T	T
6.9719440640425843	6.4798434089298595	18.1341818727142901	T	T	T
5.6647057109386161	1.2568929929220687	19.3779451917586236	T	T	T
1.9339905510459159	6.5398463595941969	18.2434258107387244	T	T	T
1.5382164351804088	1.8037288703743863	19.7011198499532334	T	T	T
5.6335612050487018	3.6537874232871985	17.9189012139814565	T	T	T
2.0069934805258232	0.7254382793760716	20.9885857910258444	T	T	T

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  5.6632261744415091  1.0799428936482085 21.1717259608442490   T   T   T
  0.7373984900947747 -0.7812435483338078 21.5641813408958249   T   T   T
  0.7347757366087170  0.8266035863805596 23.8810958320379285   T   T   T
 -0.4751666107016913 -0.3829334201779737 25.7044858940394683   T   T   T
 -0.4784545628008757  2.2333219322972724 22.0198671685744678   T   T   T
  0.7544973104402070  3.3915855593227362 23.9278799502071600   T   T   T
 -0.4767848762203309  2.1345940700348720 25.7087171329202739   T   T   T
 -0.4833912351998090  4.7237203024593484 22.1975438881251854   T   T   T
  0.8020028907247423  5.9514050823953584 23.8965259043568778   T   T   T
 -0.4833190800317002  4.6828580458807778 25.7064427355093308   T   T   T
  3.2873285542196480 -0.8081312744865526 21.4896721756863869   T   T   T
  3.3385088981235804  0.8302020040563957 23.9296625314968274   T   T   T
  2.0451479156666665 -0.3794764148816838 25.7023517978009508   T   T   T
  2.0586011996198303  2.1344122991839041 22.3338715158123371   T   T   T
  3.3185739861518866  3.4189842781327027 23.9612724728031097   T   T   T
  2.0419675424212143  2.1250621489891834 25.6946926219691782   T   T   T
  2.0444991926956990  4.6510273037850141 22.1659225022998605   T   T   T
  3.2972150569025089  5.9709844929149209 23.8800762981256796   T   T   T
  2.0433201516666792  4.6771588047371830 25.7040133914651321   T   T   T
  5.7957741675252423 -0.8974569622072468 21.4474529507953200   T   T   T
  5.8481002391336441  0.8812616546739093 23.8884208176116353   T   T   T
  4.5800529336940299 -0.3778460776804649 25.7036173809747019   T   T   T
  4.5177677067580051  2.2217388363791377 22.2025970985719212   T   T   T
  5.8444242249697478  3.4090625416228364 23.9275388321003533   T   T   T
  4.5779682830961290  2.1396322121383893 25.7125191509820148   T   T   T
  4.5761520117364869  4.7137381549913675 22.2125057748308876   T   T   T
  5.8362724353040729  6.0114222671267719 23.8771705447185134   T   T   T
  4.5848217951661576  4.6891729922855649 25.7049290177821383   T   T   T
  0.7878897827294831  0.8802973058836867 27.5142985729642753   T   T   T
 -0.4700096511260430 -0.3788864325732556 29.2933164950751532   T   T   T
  0.7867759394637905  3.4036364437064797 27.4909640485062425   T   T   T
 -0.4695269840938761  2.1460527313385733 29.2823060708962757   T   T   T
  0.7880937301264128  5.9326744781942509 27.5079752460032552   T   T   T
 -0.4723151550986270  4.6672146086615083 29.2751078519713879   T   T   T
  3.3141609297901193  0.8826494111573703 27.5124698053610146   T   T   T
  2.0520737679115686 -0.3789397763133192 29.2865155808774240   T   T   T
  3.3111505542064892  3.4064657124658795 27.4851445064281172   T   T   T
  2.0535923966453025  2.1463983546063585 29.2753512624611361   T   T   T
  3.3120601257842153  5.9359502242548867 27.5009403465654110   T   T   T
  2.0504088538724186  4.6680729816951629 29.2633326272843171   T   T   T
  5.8383552999608597  0.8803391071318460 27.5183644668400653   T   T   T
  4.5728877402191825 -0.3761264843522426 29.2903664456478339   T   T   T
  5.8364513068120676  3.4098076170964511 27.5042532939546511   T   T   T
  4.5755682560850426  2.1490319662568118 29.2786487940762292   T   T   T
  5.8361520954899699  5.9358053089356764 27.5173224973584958   T   T   T
  4.5695059882532183  4.6702537268351714 29.2712898147865097   T   T   T

Oxide reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Cu E_tot= -678.10123645 eV
 D3-zero damping= -12.4730346 eV, D3-BJ damping= -18.9031813 eV
 O Al  O Al  O Al  H  O  H  O  H
 1.0000000000000000
     7.5713089101900026    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.5713089101900026    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6840463963622163
  18  12  24  16  12   8   1   1   1   1   2
Selective dynamics
Cartesian
  3.0742706814383642  6.7965354071552930 10.9423958550990683   F   F   F
  6.9496160755450562  4.6461529487152262  9.3854545373318210   F   F   F
  3.0752007950165097  6.4675089756823914  8.0000187449185951   F   F   F
  3.1643082791158981  2.9204295489932952  8.1990827428381010   F   F   F
  6.8608430427428830  1.0991113643589845  9.5845317789161726   F   F   F
  3.1579568896376000  2.7472501105824416 10.8220669229527680   F   F   F
```

0.6167580046523641	2.9205028833781403	8.1993257849376384	F	F	F
4.4914896717292514	1.0990167280483447	9.5846030099037201	F	F	F
0.6234568781037551	2.7471348797031352	10.8217845066302907	F	F	F
0.7068216598067383	6.7966335472545181	10.9423584978630899	F	F	F
4.4019571249731957	4.6462339086007374	9.3853700880230981	F	F	F
0.7058030603129238	6.4672753136124310	8.0000000000000000	F	F	F
5.6759218341858286	6.6332349909229507	10.9172067463060003	F	F	F
5.6758822732918386	6.7313330050628108	8.0327436308783255	F	F	F
1.8908285973753074	0.8351705312417778	9.5519775531218265	F	F	F
1.8907256769869536	4.8451065823013115	9.4220834377914784	F	F	F
5.6760058693227018	2.7213904474369603	8.1626394660302282	F	F	F
5.6760812370181952	2.8156935438133313	10.8301543211852653	F	F	F
0.5684923931206077	4.6410324770634208	8.0560139425344559	F	F	F
4.3541726304528670	2.9256773813273207	9.5285274732362595	F	F	F
0.5945048895347544	1.0367489316290468	10.9191009939757393	F	F	F
6.9979689459477150	2.9256281990931861	9.5284873332419124	F	F	F
3.1864724694090163	1.0368047279410977	10.9192047381793635	F	F	F
3.2123063240941336	4.6409616849872153	8.0559839586400095	F	F	F
5.6757780022636899	0.9494924830044873	8.1168144920444938	F	F	F
5.6761137094586616	0.9487371739588352	10.8835529458276739	F	F	F
5.6758398312500882	5.6436288270516490	9.4463612987341463	F	F	F
1.8908929283971920	6.6170420180407037	9.4677862360962415	F	F	F
1.8905788580977576	1.9229954669488631	8.1383270166926529	F	F	F
1.8906804002363682	3.7751923370469673	10.8469192662674665	F	F	F
3.0846807772878013	6.7322992999401441	16.7695625120899656	T	T	T
6.9979707787298526	4.6867865451371982	15.0258774870970377	T	T	T
3.0752007950165097	6.4675089756823914	13.5580397357678457	F	F	F
6.9431163702665497	4.8192064301244377	12.3205669558782276	F	F	F
6.8596658874772460	0.7701121542613976	12.2001224306209899	F	F	F
3.1643082791158981	2.9204295489932952	13.7571037336873516	F	F	F
6.9334128992681023	0.9954000427686913	15.1953686897679869	T	T	T
3.1799823618459202	2.7991229605289170	16.5056767436312164	T	T	T
4.4921781666780438	0.7700394595828238	12.2001609218852352	F	F	F
0.6167580046523641	2.9205028833781403	13.7573467757868890	F	F	F
4.4273372213910376	0.9973430604270310	15.1968141291142160	T	T	T
0.5794653326245663	2.8072095520088731	16.5345300995985767	T	T	T
0.7417313347621093	6.7427507299593339	16.7876155276351611	T	T	T
4.3572054602930885	4.6935382625965270	15.0247500712933348	T	T	T
0.7058030603129238	6.4672753136124310	13.5580209908492506	F	F	F
4.4086996711235455	4.8191266125708356	12.3204488991888077	F	F	F
5.6911736278859930	6.5979064455908221	16.6349882422404001	T	T	T
5.6758822732918386	6.7313330050628108	13.5907646217275762	F	F	F
1.8905265783182470	0.9333255642403494	12.2256103096605884	F	F	F
1.8882923183383253	0.8592049225022133	15.2514890214417598	T	T	T
1.8895719756157576	4.8378620866004223	15.0608070463143289	T	T	T
1.8906033418294066	4.7507750788174317	12.3122395822918378	F	F	F
5.6760058693227018	2.7213904474369603	13.7206604568794788	F	F	F
5.6792030571532663	2.7656821173957695	16.3962798488539612	T	T	T
0.5684923931206077	4.6410324770634208	13.6140349333837065	F	F	F
4.3800115540927473	6.5296561451253972	12.2234202596149437	F	F	F
4.3286800196214053	2.9159455910490704	15.1391583672140513	T	T	T
0.6175747886688746	1.0515948610339521	16.6903476061372480	T	T	T
7.0258725068038315	2.9065860355141879	15.1337365894790370	T	T	T
3.1607426377913779	1.0485525466038175	16.6590825456015956	T	T	T
3.2123063240941336	4.6409616849872153	13.6140049494892601	F	F	F
6.9719322530726959	6.5297105535807285	12.2233730105456431	F	F	F
5.6757780022636899	0.9494924830044873	13.6748354828937444	F	F	F
5.6811065789135844	0.8818617561942335	16.5144760852383996	T	T	T
5.6808544867062309	5.7573444815616162	15.0893170644414738	T	T	T
1.8901274384868614	6.6184213545717530	15.1584836452566147	T	T	T
1.8904629143660816	6.6180150951668049	12.2590327337071869	F	F	F
1.8905788580977576	1.9229954669488631	13.6963480075419035	F	F	F
1.8871541675546868	3.9200037629027662	16.5844953032411979	T	T	T

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  5.6759058834275962  3.7912082295675131 12.2955930440659955   F   F   F
  3.2445595310896351  6.3024529807239942 19.4359807626005363   T   T   T
  6.9944201288246814  4.7078431882047527 18.0547718538448123   T   T   T
  6.8846124595514313  0.8613480418430084 17.9244081142316318   T   T   T
  3.1678808250166997  3.0906070936917245 20.2655908762925883   T   T   T
  4.4376285972499092  0.8820326272186801 17.9094046638853399   T   T   T
  0.5004433580943121  3.1185174403700264 20.2120127830484755   T   T   T
  0.6341171486880771  6.3830996808321716 19.4868672614133835   T   T   T
  4.4610067792944950  4.6082658768011573 18.0376613461906992   T   T   T
  5.6959542723012300  6.7201654318792663 19.2934394891934353   T   T   T
  1.8885694595811833  1.0706603935631274 18.1849012662558849   T   T   T
  1.9312946443841879  4.5462785007473006 18.2329822734576226   T   T   T
  5.8444656379292015  2.6407946514482519 19.4973588640161815   T   T   T
  0.5455453657824133  4.6185365573545853 19.3573510428248383   T   T   T
  4.4354688139118297  6.4117097195356214 18.0016731599670514   T   T   T
  3.3593434939676290  4.5168558832776862 19.3543138596910431   T   T   T
  6.9744564788706054  6.5199327764375994 18.0462426297001777   T   T   T
  5.4865761067664636  0.8975472971880489 19.3790212328381060   T   T   T
  1.9373442244392662  6.7547299300729673 18.3008380443586276   T   T   T
  1.8418618086335279  1.9764363732667616 19.9028496036585487   T   T   T
  5.7737254827758502  3.5228478931439233 17.9542629630875119   T   T   T
  6.8513022638849712  2.8008887192321836 19.9421110116796143   T   T   T
  1.9225085203423136  0.7008823669658643 21.0790583047871820   T   T   T
  1.4502856231127719 -0.1236112444974025 20.8467800498283680   T   T   T
  4.5417870269385494  1.0189740717256079 20.9832860875475546   T   T   T
  4.1875691365715175  1.9734130217069341 20.9642070970302896   T   T   T
  3.6814594868522050  0.4965075390278342 21.0961112142999347   T   T   T

Metal reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Cu E_tot= -173.98184631 eV
 D3-zero damping= -16.8611412 eV, D3-BJ damping= -20.3780334 eV
Cu
 1.0000000000000000
     7.5713089101900026    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.5713089101900026    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0001559791606477 -0.0001563790284090  8.2531365685509641
  1.2619378323209398  1.2619375981006291 10.0242949591771566
 -0.0004063062167627 -0.0004063704229356 11.8276157489577916
  1.2616054292823389  1.2616055741405616 13.6312266804165656
 -0.0007399052426475 -0.0007396623845194 15.4025494126481295
 -0.0001686103269882  2.5232484381304197  8.2527595471933761
  1.2618696147409953  3.7853694565799700 10.0239414806670837
 -0.0004602357656926  2.5228570519187379 11.8275487974655409
  1.2615050351894372  3.7849893617214798 13.6314906343159770
 -0.0008100095988099  2.5227253726391883 15.4029435579470899
 -0.0001614081217112  5.0477400200425118  8.2527662706308327
  1.2619262122153880  6.3088348085377479 10.0242902633812516
 -0.0004621917150900  5.0475849334381016 11.8275558915558250
  1.2615874056631262  6.3084712697320766 13.6311672322289734
 -0.0008020332643568  5.0471719978963048 15.4028927199030310
  2.5232487966725694 -0.0001690284560401  8.2527595471933761
  3.7853696606272274  1.2618691962840287 10.0239414029962095
  2.5228571045061132 -0.0004601549088411 11.8275488157268303
  3.7849891660070987  1.2615052529052411 13.6314905621286435
  2.5227251819351508 -0.0008096954184889 15.4029435579470899
  2.5230533828103936  2.5230530719321145  8.2523450237744935
  3.7853780238854244  3.7853775516870192 10.0233021369657642
  2.5229972569386740  2.5229973267832593 11.8274970264182269
  3.7849736189709509  3.7849739019951194 13.6320275080877398
  2.5225065726209701  2.5225068267851767 15.4033327417629913
  2.5230529200473897  5.0479261121161345  8.2523530227240940
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  3.7853713796963366  6.3088788069057697 10.0239140941770923
  2.5229740513414893  5.0474803400900452 11.8274927687177804
  3.7849929777958331  6.3084802598539955 13.6314159874857186
  2.5225038986044921  5.0473588501023503 15.4032685334809081
  5.0477403110716459 -0.0001619528299373  8.2527664067188251
  6.3088350069159995  1.2619258332322529 10.0242902172011945
  5.0475849023970722 -0.0004621753603053 11.8275558858868255
  6.3084709974401738  1.2615876285602672 13.6311671543283257
  5.0471717693820271 -0.0008016461524593 15.4028927055591875
  5.0479263553092810  2.5230525043766474  8.2523529959808233
  6.3088790654110456  3.7853709335689403 10.0239139942556026
  5.0474803035183022  2.5229740101384666 11.8274927687177804
  6.3084800641396130  3.7849932062237115 13.6314159247075253
  5.0473586302403328  2.5225042103183655 15.4032683622334012
  5.0479345074322346  5.0479341625935881  8.2523438779395590
  6.3088448741306662  6.3088445895543890 10.0242871343149389
  5.0474931046530571  5.0474932524176923 11.8274913241470347
  6.3084910976839188  6.3084913059905903 13.6311069154961402
  5.0473671385732413  5.0473673794631546 15.4032329402729857

Interface: 2O-g-Al2O3(110)/fcc(100)_3x3/Pt E_tot= -965.3322991 eV
 D3-zero damping= -40.6852098 eV, D3-BJ damping= -46.3465011 eV
 O Al  O Al  O Al  O Pt
 1.0000000000000000
     8.3113600962600014    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.3113600962600014    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.2716937760818396
  18  12  24  16  12   8   2  45
Selective dynamics
Cartesian
  3.3747626691627945  7.4608570124278737 10.9423958550990683   F   F   F
  7.6289004212829958  5.1002872392513972  9.3854545373318210   F   F   F
  3.3757836959060024  7.0996701706813692  8.0000187449185951   F   F   F
  3.4736009156769483  3.2058844653364353  8.1990827428381010   F   F   F
  7.5314503434684532  1.2065430751061383  9.5845317789161726   F   F   F
  3.4666287150057160  3.0157777491828393 10.8220669229527680   F   F   F
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Oxide reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Pt E_tot= -693.86870551 eV
 D3-zero damping= -10.6546535 eV, D3-BJ damping= -16.0700861 eV
 O Al  O Al  O Al  H  O  H  O  H
 1.0000000000000000
     8.3113600962600014    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.3113600962600014    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6840463963622163
  18  12  24  16  12   8   1   1   1   1   2
Selective dynamics
Cartesian
  3.3747626691627945  7.4608570124278737 10.9423958550990683   F   F   F
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  4.8608619410347496  7.0941387661730184 17.8076714330140256   T   T   T
  3.5460511001234791  4.9833693412273750 18.8181247682896426   T   T   T
  7.6152468321156022  7.1691076681188362 17.8433804786322732   T   T   T
  6.0799393970033462  1.0354774870543857 19.0209385659988470   T   T   T
  2.0953557319769147  7.4735263263797291 18.0171575578381926   T   T   T
  2.0619311548343222  2.3202861938560355 19.4249632380565593   T   T   T
  6.2873394231626589  4.0473373026573443 17.7738381389028355   T   T   T
  7.5678871516029700  3.0051532603503923 19.3915654657597578   T   T   T
  2.2893266584886773  1.0999760981647002 20.6687604682717456   T   T   T
  1.7852159342040925  0.2698022140941801 20.6759976174433078   T   T   T
  4.9360975097435622  1.3954729321396993 20.4674810537577301   T   T   T
  4.5639314447307644  2.3321761433918042 20.3026904830765176   T   T   T
  4.0822461728785715  0.8874484376365656 20.6375480392806345   T   T   T

Metal reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Pt E_tot= -284.83068848 eV
 D3-zero damping= -26.2261496 eV, D3-BJ damping= -26.788886 eV
Pt
 1.0000000000000000
     8.3113600962600014    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.3113600962600014    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0002044765405899 -0.0002052706292012  7.9297751302158259
  1.3851874200727903  1.3851868271119350  9.8759158461155288
 -0.0000789564021926 -0.0000790434411963 11.8275971545169813
  1.3844598001513646  1.3844602327809783 13.7795168648150987
 -0.0013794526760332 -0.0013785925153213 15.7257940782513437
 -0.0002044704573649  2.7702481277041540  7.9297750776975731
  1.3851874584032424  4.1556402746949885  9.8759158674847267
 -0.0000790126971761  2.7703744108857884 11.8275971785238116
  1.3844597903451614  4.1549135930138101 13.7795169273632698
 -0.0013794570870213  2.7690747606121153 15.7257941575337181
 -0.0002044765405899  5.5407014816328939  7.9297750743555797
  1.3851874055358107  6.9260935368843857  9.8759158376617666
 -0.0000789763343884  5.5408277514083295 11.8275971544105563
  1.3844597618209131  6.9253669194255805 13.7795168650259701
 -0.0013794740671052  5.5395281433485488 15.7257940853902323
  2.7702489115747184 -0.0002051606745426  7.9297750902131376
  4.1556407447508850  1.3851868315229232  9.8759158630020085
  2.7703744006519400 -0.0000790194124838 11.8275971221442848
  4.1549131329634328  1.3844601988615139 13.7795168841839679
  2.7690738543233322 -0.0013785925153213 15.7257940796883435
  2.7702489698373651  2.7702481776228187  7.9297750139014145
  4.1556408194122572  4.1556402471328013  9.8759158477658975
  2.7703744338005380  2.7703744254227680 11.8275971446043524
  4.1549131415426563  4.1549135728388595 13.7795169065404366
  2.7690739509164306  2.7690747606121153 15.7257942332325609
  2.7702489499051697  5.5407015155523558  7.9297749760902381
  4.1556406933952275  6.9260935179364163  9.8759157827857589
  2.7703744410788711  5.5408277692473860 11.8275971819727417
  4.1549131317364507  6.9253669286820729 13.7795169351901592
  2.7690738866960296  5.5395281433485488 15.7257940741733684
  5.5407022698743731 -0.0002051864766026  7.9297751177753248
```

```
  6.9260941207257849  1.3851868478997640  9.8759158685969712
  5.5408277446989009 -0.0000790646499239 11.8275971185889333
  6.9253664723737192  1.3844602042567304 13.7795168886085708
  5.5395272876338169 -0.0013786284433729 15.7257941106240420
  5.5407022698743731  2.7702481117301794  7.9297750702809413
  6.9260941277932453  4.1556402427218107  9.8759158606306325
  5.5408277762990412  2.7703743978605804 11.8275971683978245
  6.9253664637944947  4.1549136111693121 13.7795168904916849
  5.5395272876338169  2.7690747496304882 15.7257940967432113
  5.5407022458456616  5.5407014233702458  7.9297750419828823
  6.9260940823953332  6.9260935223474061  9.8759157783611560
  5.5408277465606437  5.5408276968686625 11.8275971819727417
  6.9253664848175527  6.9253669108463551 13.7795168791387148
  5.5395272876338169  5.5395280755941663 15.7257941164620458

Interface: 2O-g-Al2O3(110)/fcc(100)_3x3/Pd E_tot= -922.69204881 eV
 D3-zero damping= -34.2598384 eV, D3-BJ damping= -42.8172778 eV
 O Al  O Al  O Al  O Pd
 1.0000000000000000
     8.2439436957000023    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.2439436957000023    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.2976501681054629
  18  12  24  16  12   8   2  45
Selective dynamics
Cartesian
  3.3473887677478400  7.4003393451573807 10.9423958550990683   F   F   F
  7.5670196941003303  5.0589169937668892  9.3854545373318210   F   F   F
  3.3484015125796511  7.0420822184657137  8.0000187449185951   F   F   F
  3.4454253020583985  3.1798803951528498  8.1990827428381010   F   F   F
  7.4703600685588762  1.1967563746982413  9.5845317789161726   F   F   F
  3.4385096553888932  2.9913157022513954 10.8220669229527680   F   F   F
  0.6715507615048258  3.1799602445615576  8.1993257849376384   F   F   F
  4.8905134373423458  1.1966533309014900  9.5846030099037201   F   F   F
  0.6788447626099137  2.9911902342653081 10.8217845066302907   F   F   F
  0.7696156682374413  7.4004462040191576 10.9423584978630899   F   F   F
  4.7930268226572466  5.0590051461254415  9.3853700880230981   F   F   F
  0.7685065764046971  7.0418277978666568  8.0000000000000000   F   F   F
  6.1801705064822157  7.2225313263758544 10.9172067463060003   F   F   F
  6.1801274309999608  7.3293443642299252  8.0327436308783255   F   F   F
  2.0588097355269928  0.9093670483578636  9.5519775531218265   F   F   F
  2.0586976716953895  5.2755456603282509  9.4220834377914784   F   F   F
  6.1802620072973404  2.9631586676501263  8.1626394660302282   F   F   F
  6.1803440706559343  3.0658396473960003 10.8301543211852653   F   F   F
  0.6189972349447344  5.0533416196151224  8.0560139425344559   F   F   F
  4.7409971555249371  3.1855944447048308  9.5285274732362595   F   F   F
  0.6473206805162403  1.1288536658996928 10.9191009939757393   F   F   F
  7.6196682316059796  3.1855408931229516  9.5284873332419124   F   F   F
  3.4695585581445858  1.1289144191539098 10.9192047381793635   F   F   F
  3.4976874914628877  5.0532645383736545  8.0559839586400095   F   F   F
  6.1800138965377762  1.0338453578144855  8.1168144920444938   F   F   F
  6.1803794279467335  1.0330229471429531 10.8835529458276739   F   F   F
  6.1800812184088922  6.1450085898655633  9.4463612987341463   F   F   F
  2.0588797817143289  7.2048997704202415  9.4677862360962415   F   F   F
  2.0585378094218574  2.0938343085271010  8.1383270166926529   F   F   F
  2.0586483725600648  4.1105802756464582 10.8469192662674665   F   F   F
  3.3275153177445405  7.4199703011444411 16.5578919035138554   T   T   T
  7.5684766612126015  5.0309664698336327 14.9456293957912489   T   T   T
  3.3484015125796511  7.0420822184657137 13.5580397357678457   F   F   F
  7.5599425552607658  5.2473445396516336 12.3205669558782276   F   F   F
  7.4690783348657828  0.8385288877277990 12.2001224306209899   F   F   F
  3.4454253020583985  3.1798803951528498 13.7571037336873516   F   F   F
  7.4763259053547184  1.1899606651451140 15.0807429440571639   T   T   T
  3.4436684240505735  2.9607222075630317 16.3739963168588254   T   T   T
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4.8912630981552843	0.8384497348568426	12.2001609218852352	F	F	F
0.6715507615048258	3.1799602445615576	13.7573467757868890	F	F	F
4.8743356548930148	1.1897209361864884	15.0930499385195898	T	T	T
0.6716321152125693	2.9546605699305997	16.3652772595205960	T	T	T
0.7890631435146654	7.4045473504664852	16.5432420672930895	T	T	T
4.7927808241422474	5.0297981908303093	14.9434238230869010	T	T	T
0.7685065764046971	7.0418277978666568	13.5580209908492506	F	F	F
4.8003683763421492	5.2472576311097123	12.3204488991888077	F	F	F
6.1754570435806126	7.2104390762526087	16.4210240823740570	T	T	T
6.1801274309999608	7.3293443642299252	13.5907646217275762	F	F	F
2.0584808851087932	1.0162421706238094	12.2256103096605884	F	F	F
2.0602062161200463	0.8927339395581343	15.0861296247829255	T	T	T
2.0606326614330510	5.2727005287677642	14.9695630467520271	T	T	T
2.0585644682872624	5.1728337497885555	12.3122395822918378	F	F	F
6.1802620072973404	2.9631586676501263	13.7206604568794788	F	F	F
6.1779705907572913	3.0247186301868005	16.3511850740889777	T	T	T
0.6189972349447344	5.0533416196151224	13.6140349333837065	F	F	F
4.7691316081237431	7.1097505399953924	12.2234202596149437	F	F	F
4.7529564150429140	3.1792565336592680	15.0729932670440672	T	T	T
0.6445022416585745	1.1026471037950649	16.4101858524130186	T	T	T
7.6038364274083019	3.1798988575443303	15.0735030590583392	T	T	T
3.4778276871679759	1.1131793705780557	16.4469712287418304	T	T	T
3.4976874914628877	5.0532645383736545	13.6140049494892601	F	F	F
7.5913184399609710	7.1098097820957546	12.2233730105456431	F	F	F
6.1800138965377762	1.0338453578144855	13.6748354828937444	F	F	F
6.1737743043538602	0.9798871295507564	16.3743152307100779	T	T	T
6.1797003960380064	6.1247653797357078	14.9864601945944642	T	T	T
2.0607562742291314	7.1811689273545412	15.0904570196184835	T	T	T
2.0584115652536239	7.2059592956799170	12.2590327337071869	F	F	F
2.0585378094218574	2.0938343085271010	13.6963480075419035	F	F	F
2.0546124529565812	4.0601932798099485	16.3267284781308213	T	T	T
6.1801531386592492	4.1280190194280078	12.2955930440659955	F	F	F
3.4228883209375294	6.8443258065103034	19.0764265492260776	T	T	T
7.4611278556002425	5.1812682937923897	17.8706621061551090	T	T	T
7.5037230369385428	0.8374066701358632	17.6434551005237026	T	T	T
3.3946902061213087	3.3001736016496896	19.4141002070158848	T	T	T
4.8798357061927407	0.8493729165286548	17.7023669262376799	T	T	T
0.6773114207862930	3.2802760937300288	19.4049153126148077	T	T	T
0.6643747420102678	6.8423270744797149	19.0643454391181031	T	T	T
4.8610134463811896	5.1998131225572335	17.8552490468883320	T	T	T
6.1526044802382227	7.3939716549338685	19.0326516234269327	T	T	T
2.0491157624883853	1.0769280638958150	17.7411744531370559	T	T	T
2.0433255841270883	5.0384990384254307	17.8235491663770418	T	T	T
6.1004403653667802	2.8722427871328771	19.2070088654351245	T	T	T
0.5855750863014448	4.9790763281610486	18.9342687209312999	T	T	T
4.8030853290759854	7.0829696750702738	17.8054617753594897	T	T	T
3.5031053811660002	4.9903960313827485	18.9276685240503575	T	T	T
7.5322537642028813	7.0552360964140410	17.7973394262761637	T	T	T
6.3095757504086203	1.0819732612276072	19.0434627839838981	T	T	T
2.0452156449087311	7.4034047593346672	18.0220827789426785	T	T	T
2.0447189276205133	2.1900000667631838	19.1880926024518104	T	T	T
6.1502020959944161	4.0006906230248642	17.8715516729407646	T	T	T
2.1358199321068549	0.7939905728707575	20.2457418923676684	T	T	T
7.4759336400988063	0.9369867283030612	20.3950589167980532	T	T	T
0.7099170568285269	0.8032893405957101	21.6700122680665359	T	T	T
2.0493907448987358	2.2507543582491412	23.5321733342169566	T	T	T
0.6694752799052484	0.8509949809157165	25.4475217824235642	T	T	T
0.6332214739954325	3.6323423244518720	21.4965799802976107	T	T	T
2.0438022321742402	4.9897626921519889	23.4227915396457149	T	T	T
0.6647119337101700	3.6295661183628787	25.4216435473527405	T	T	T
0.6659345255876867	6.3048384768001062	21.3533987683326494	T	T	T
2.0530800775061606	7.6802844551952862	23.5193075340261331	T	T	T
0.6638639276644482	6.3288982307210588	25.4258365642696837	T	T	T

```
  3.5256005126363483  0.8349524624450624 21.6595652220128407   T   T   T
  4.7895084487583643  2.2794408035148996 23.5429733682878179   T   T   T
  3.4184556570764961  0.8531921925091109 25.4549833986785963   T   T   T
  3.4613011129505145  3.6219577500006537 21.4956402357378629   T   T   T
  4.8123600962459552  4.9970703254118849 23.3828292684995560   T   T   T
  3.4164388973173305  3.6288375695963180 25.4294934657771421   T   T   T
  3.4351016395687037  6.3431841729131602 21.3512324266323859   T   T   T
  4.7900779730898595  7.6806383878732811 23.5303845889927494   T   T   T
  3.4182886325227457  6.3333297112496689 25.4337951219011842   T   T   T
  6.0761648726891844  0.8598212023465434 21.7540503321655088   T   T   T
  7.5465350119888699  2.2726821970634519 23.5268262098772851   T   T   T
  6.1696495218280587  0.8574896794980840 25.4446393033657827   T   T   T
  6.1540744909301530  3.6365699001316210 21.2808804949325534   T   T   T
  7.5061714961144341  4.9890881354299541 23.3760965531987992   T   T   T
  6.1670967013048532  3.6361446802329027 25.4282948019190798   T   T   T
  6.1651473347463588  6.3896150659271012 21.2462620491990428   T   T   T
  7.5507523531389049  7.6704469976734773 23.5164875077441877   T   T   T
  6.1664793460842375  6.3343137802263954 25.4321976780228702   T   T   T
  2.0409349589150363  2.2352006708830676 27.3783842124102463   T   T   T
  0.6681668283088373  0.8597115643454482 29.3292981530109813   T   T   T
  2.0387312214350035  4.9786534699195544 27.3824714004762306   T   T   T
  0.6693400363827401  3.6044033318475512 29.3345379236166366   T   T   T
  2.0413495045940073  7.7224847958592857 27.3844787693348941   T   T   T
  0.6678132114228784  6.3534285314574239 29.3371767689087442   T   T   T
  4.7917544137489383  2.2381639390972135 27.3789633264345049   T   T   T
  3.4206165324786393  0.8586876465339928 29.3311008937244146   T   T   T
  4.7898540867088997  4.9815530773575842 27.3878362043974413   T   T   T
  3.4159494637881345  3.6019733850866613 29.3308974859954716   T   T   T
  4.7931257019768170  7.7235480140232289 27.3846260595219633   T   T   T
  3.4138156949889353  6.3551331064865106 29.3340206158814851   T   T   T
  7.5410973372012862  2.2361497766612199 27.3771884780813828   T   T   T
  6.1630621627056934  0.8613461270526042 29.3320548776490071   T   T   T
  7.5391304024738739  4.9805243797537990 27.3891965545531590   T   T   T
  6.1648375169327894  3.6028942211165451 29.3306631983145536   T   T   T
  7.5411463360644388  7.7240947158521776 27.3829110801540700   T   T   T
  6.1650676952734251  6.3600929240721955 29.3361088376039376   T   T   T

Oxide reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Pd E_tot= -694.3302536 eV
 D3-zero damping= -10.8307585 eV, D3-BJ damping= -16.3093253 eV
 O Al  O Al  O Al  H  O  H  O  H
 1.0000000000000000
     8.2439436957000023    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.2439436957000023    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6840463963622163
  18  12  24  16  12   8   1   1   1   1   2
Selective dynamics
Cartesian
  3.3473887677478400  7.4003393451573807 10.9423958550990683   F   F   F
  7.5670196941003303  5.0589169937668892  9.3854545373318210   F   F   F
  3.3484015125796511  7.0420822184657137  8.0000187449185951   F   F   F
  3.4454253020583985  3.1798803951528498  8.1990827428381010   F   F   F
  7.4703600685588762  1.1967563746982413  9.5845317789161726   F   F   F
  3.4385096553888932  2.9913157022513954 10.8220669229527680   F   F   F
  0.6715507615048258  3.1799602445615576  8.1993257849376384   F   F   F
  4.8905134373423458  1.1966533309014900  9.5846030099037201   F   F   F
  0.6788447626099137  2.9911902342653081 10.8217845066302907   F   F   F
  0.7696156682374413  7.4004462040191576 10.9423584978630899   F   F   F
  4.7930268226572466  5.0590051461254415  9.3853700880230981   F   F   F
  0.7685065764046971  7.0418277978666568  8.0000000000000000   F   F   F
  6.1801705064822157  7.2225313263758544 10.9172067463060003   F   F   F
  6.1801274309999608  7.3293443642299252  8.0327436308783255   F   F   F
  2.0588097355269928  0.9093670483578636  9.5519775531218265   F   F   F
  2.0586976716953895  5.2755456603282509  9.4220834377914784   F   F   F
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6.1802620072973404	2.9631586676501263	8.1626394660302282	F	F	F
6.1803440706559343	3.0658396473960003	10.8301543211852653	F	F	F
0.6189972349447344	5.0533416196151224	8.0560139425344559	F	F	F
4.7409971555249371	3.1855944447048308	9.5285274732362595	F	F	F
0.6473206805162403	1.1288536658996928	10.9191009939757393	F	F	F
7.6196682316059796	3.1855408931229516	9.5284873332419124	F	F	F
3.4695585581445858	1.1289144191539098	10.9192047381793635	F	F	F
3.4976874914628877	5.0532645383736545	8.0559839586400095	F	F	F
6.1800138965377762	1.0338453578144855	8.1168144920444938	F	F	F
6.1803794279467335	1.0330229471429531	10.8835529458276739	F	F	F
6.1800812184088922	6.1450085898655633	9.4463612987341463	F	F	F
2.0588797817143289	7.2048997704202415	9.4677862360962415	F	F	F
2.0585378094218574	2.0938343085271010	8.1383270166926529	F	F	F
2.0586483725600648	4.1105802756464582	10.8469192662674665	F	F	F
3.3325895631722724	7.4417899891495525	16.5638523373511077	T	T	T
7.5659117482498468	5.0231384815434170	14.9487650901914915	T	T	T
3.3484015125796511	7.0420822184657137	13.5580397357678457	F	F	F
7.5599425552607658	5.2473445396516336	12.3205669558782276	F	F	F
7.4690783348657828	0.8385288877277990	12.2001224306209899	F	F	F
3.4454253020583985	3.1798803951528498	13.7571037336873516	F	F	F
7.4869173381334031	1.1813177160600383	15.0944803909544412	T	T	T
3.4498398798591059	2.9591638957037745	16.3681798680328292	T	T	T
4.8912630981552843	0.8384497348568426	12.2001609218852352	F	F	F
0.6715507615048258	3.1799602445615576	13.7573467757868890	F	F	F
4.8777578508506831	1.1860081942804603	15.0884214882378238	T	T	T
0.6507736531294362	2.9578782877363778	16.3822673451600345	T	T	T
0.8070133559307289	7.4358327756534868	16.5693479431275286	T	T	T
4.7927807365534800	5.0265073871924884	14.9497841348777900	T	T	T
0.7685065764046971	7.0418277978666568	13.5580209908492506	F	F	F
4.8003683763421492	5.2472576311097123	12.3204488991888077	F	F	F
6.1696553597558026	7.2126292586977740	16.4345074986249209	T	T	T
6.1801274309999608	7.3293443642299252	13.5907646217275762	F	F	F
2.0584808851087932	1.0162421706238094	12.2256103096605884	F	F	F
2.0559462955705778	0.9160957261321724	15.1216693286769885	T	T	T
2.0563401654913012	5.2769682597719338	14.9644216795849534	T	T	T
2.0585644682872624	5.1728337497885555	12.3122395822918378	F	F	F
6.1802620072973404	2.9631586676501263	13.7206604568794788	F	F	F
6.1805646353182953	3.0130732845776378	16.3223594905312623	T	T	T
0.6189972349447344	5.0533416196151224	13.6140349333837065	F	F	F
4.7691316081237431	7.1097505399953924	12.2234202596149437	F	F	F
4.7544788286830766	3.1672060435815204	15.0581773543873361	T	T	T
0.6490656303039497	1.1197617371200084	16.4916067597851246	T	T	T
7.6050584208702796	3.1614301294863121	15.0531264958209672	T	T	T
3.4566108532948130	1.1271097973602564	16.4639273248387568	T	T	T
3.4976874914628877	5.0532645383736545	13.6140049494892601	F	F	F
7.5913184399609710	7.1098097820957546	12.2233730105456431	F	F	F
6.1800138965377762	1.0338453578144855	13.6748354828937444	F	F	F
6.1833541577519799	0.9556858271862412	16.3654744749620384	T	T	T
6.1807586566361037	6.1270856669133460	14.9862063087753690	T	T	T
2.0553980238042344	7.1973356112052747	15.0907304530495896	T	T	T
2.0584115652536239	7.2059592956799170	12.2590327337071869	F	F	F
2.0585378094218574	2.0938343085271010	13.6963480075419035	F	F	F
2.0521473942680948	4.0293319255136542	16.2793235855461269	T	T	T
6.1801531386592492	4.1280190194280078	12.2955930440659955	F	F	F
3.4455538894499331	6.7651402652869939	19.0653923062279205	T	T	T
7.4941686740195514	5.2205356412602342	17.8445311615171178	T	T	T
7.4863245165109946	0.8366953529898112	17.7029881156036382	T	T	T
3.4210106364714101	3.4061296092552382	19.6533471071443060	T	T	T
4.8527588889188555	0.9099808733799496	17.6672177895683831	T	T	T
0.6553601670900308	3.4164233050238138	19.5934486447624217	T	T	T
0.7186342789820899	6.8156108584475286	19.1011908605346470	T	T	T
4.9244479527337690	5.1461392742402952	17.8539421271188701	T	T	T
6.1680764384990852	7.4579079310176528	19.0459570063156640	T	T	T

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  2.0481798286842157  1.1080321673136391 17.9004589226171831   T   T   T
  2.0802204647668505  4.9745102275014226 17.7767157720439499   T   T   T
  6.5002539581374563  2.8288163542379854 19.1322331287146810   T   T   T
  0.6463468292908485  5.0068037289608114 18.8499822939586501   T   T   T
  4.8218902952566740  7.0380197982737771 17.8194201345112866   T   T   T
  3.5278253599955272  4.9440623000113986 18.8587243397197284   T   T   T
  7.5571852273970803  7.1134146120419190 17.8545825659503876   T   T   T
  6.0313173290047288  1.0265637175872622 19.0463800920812538   T   T   T
  2.0813013117352188  7.4053184915519621 18.0350407392858259   T   T   T
  2.0422658308378181  2.2870124013735431 19.4555596100282493   T   T   T
  6.2400492548241173  4.0061090309111442 17.7845746302619538   T   T   T
  7.5099813685828991  2.9917491540039647 19.4295827237332261   T   T   T
  2.2564274945949609  1.0582987534519512 20.6908050153056493   T   T   T
  1.7634609914318180  0.2209856815264188 20.6714630094769980   T   T   T
  4.9006026985248123  1.3665751337719629 20.5053017590755680   T   T   T
  4.5261908869144030  2.3040345173821644 20.3486624323395731   T   T   T
  4.0489590391597927  0.8533690009046236 20.6706246063436048   T   T   T

Metal reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Pd E_tot= -241.14571846 eV
 D3-zero damping= -19.5918853 eV, D3-BJ damping= -23.0696376 eV
Pd
 1.0000000000000000
     8.2439436957000023    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.2439436957000023    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
  0.0000260702354583  0.0000253164870683  7.9394162134360498
  1.3740224950001612  1.3740219999517895  9.8879526860300739
 -0.0007555027748666 -0.0007553210314964 11.8277878496272706
  1.3735230204547353  1.3735235440453020 13.7671311508483907
 -0.0006134116074896 -0.0006125273407870 15.7165509335488789
  0.0000829262048782  2.7469414356370878  7.9362752424037435
  1.3739589260942306  4.1217298404158571  9.8853145480320599
 -0.0005568469785369  2.7488852020360532 11.8275495198548803
  1.3736256489128775  4.1210731974257708 13.7699636105038543
 -0.0009262553542314  2.7460226014490225 15.7193906407008548
  0.0000703256072604  5.4970333926063137  7.9362414408117745
  1.3739170463673822  6.8693802362022653  9.8879992027111498
 -0.0006478136546837  5.4938219068163585 11.8277650854318370
  1.3735025021983005  6.8688712936691587 13.7673316204095659
 -0.0011058698326989  5.4960717494111995 15.7191221228160938
  2.7469422352906645  0.0000821601369144  7.9362749842730507
  4.1217303832602470  1.3739583024111033  9.8853144437964460
  2.7488852330069689 -0.0005567033428515 11.8275495623189713
  4.1210727914760827  1.3736261558616372 13.7699636011410682
  2.7460218423286133 -0.0009251267037524 15.7193907101769206
  2.7476440522837970  2.7476433550061166  7.9363581934679814
  4.1216969513983326  4.1216963411507557  9.8864411826469585
  2.7476975640546661  2.7476975478895658 11.8276553033336675
  4.1213931060324729  4.1213934361976188 13.7688289030204256
  2.7468293723854105  2.7468302469662200 15.7193751831893938
  2.7476085166823001  5.4964423728692644  7.9363257832051239
  4.1216550295233834  6.8694633660418623  9.8852635374483739
  2.7476155857506255  5.4952774768685853 11.8275926095212878
  4.1211652081322701  6.8690670581859719 13.7699183759514518
  2.7468301619621882  5.4954607412217191 15.7194848898295394
  5.4970341689909805  0.0000697163292463  7.9362412014308532
  6.8693806528400403  1.3739164984687962  9.8879990757863236
  5.4938217794753097 -0.0006478318721923 11.8277650968461696
  6.8688707135137301  1.3735029046411626 13.7673315813039885
  5.4960710199865730 -0.0011049428340850 15.7191219908006037
  5.4964430624524558  2.7476077140000936  7.9363258764575964
```

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  6.8694639299798634  4.1216543814411262  9.8852635633905237
  5.4952774309303134  2.7476154593871498 11.8275924987804846
  6.8690665982062598  4.1211655266152620 13.7699182310420607
  5.4954599947578924  2.7468307621626433 15.7194847303656804
  5.4964287021820946  5.4964279154529292  7.9363211725280891
  6.8693467658444751  6.8693463159645081  9.8879825686844001
  5.4951994316315060  5.4951993249332780 11.8275495111668221
  6.8687932008664188  6.8687936662934241 13.7673598354590645
  5.4953756322081713  5.4953761785839799 15.7196055569734430

Interface: 2O-g-Al2O3(110)/fcc(100)_3x3/Ir E_tot= -1080.42551967 eV
 D3-zero damping= -38.6388959 eV, D3-BJ damping= -45.3528577 eV
 O Al  O Al  O Al  O Ir
 1.0000000000000000
     8.1451896436500029    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1451896436500029    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.2716937760818396
  18  12  24  16  12   8   2  45
Selective dynamics
Cartesian
  3.3072904583944931  7.3116908143261332 10.9423958550990683   F   F   F
  7.4763745023913755  4.9983163188278228  9.3854545373318210   F   F   F
  3.3082910715743270  6.9577252432591177  8.0000187449185951   F   F   F
  3.4041526148381629  3.1417886655575238  8.1990827428381010   F   F   F
  7.3808727607516316  1.1824204517855503  9.5845317789161726   F   F   F
  3.3973198105747153  2.9554827856932442 10.8220669229527680   F   F   F
  0.6635062671094486  3.1418675584516125  8.1993257849376384   F   F   F
  4.8319300655521626  1.1823186423485719  9.5846030099037201   F   F   F
  0.6707128935075548  2.9553588206858872 10.8217845066302907   F   F   F
  0.7603964561024460  7.3117963931275423 10.9423584978630899   F   F   F
  4.7356112412567306  4.9984034152108698  9.3853700880230981   F   F   F
  0.7593006500606559  6.9574738703598040  8.0000000000000000   F   F   F
  6.1061383560451192  7.1360127545775418 10.9172067463060003   F   F   F
  6.1060957965632854  7.2415462809879134  8.0327436308783255   F   F   F
  2.0341472910358536  0.8984737569744050  9.5519775531218265   F   F   F
  2.0340365696148570  5.2123499945203990  9.4220834377914784   F   F   F
  6.1062287607736385  2.9276630436989151  8.1626394660302282   F   F   F
  6.1063098410967482  3.0291140098502445 10.8301543211852653   F   F   F
  0.6115822782911097  4.9928077319819257  8.0560139425344559   F   F   F
  4.6842048365635867  3.1474342666135295  9.5285274732362595   F   F   F
  0.6395664378216807  1.1153311483044748 10.9191009939757393   F   F   F
  7.5283923640208785  3.1473813565250790  9.5284873332419124   F   F   F
  3.4279967790872825  1.1153911737965609 10.9192047381793635   F   F   F
  3.4557887564234040  4.9927315740952523  8.0559839586400095   F   F   F
  6.1059836221283641  1.0214609430191108  8.1168144920444938   F   F   F
  6.1063447748432020  1.0206483839901006 10.8835529458276739   F   F   F
  6.1060501375520069  6.0713976433900552  9.4463612987341463   F   F   F
  2.0342164981411819  7.1185924067110227  9.4677862360962415   F   F   F
  2.0338786223286012  2.0687523053110657  8.1383270166926529   F   F   F
  2.0339878610329807  4.0613397090583305 10.8469192662674665   F   F   F
  3.3021614297550088  7.2928963662595034 16.4775269263532209   T   T   T
  7.4882594808828111  4.9763480942261245 14.9626974618288671   T   T   T
  3.3082910715743270  6.9577252432591177 13.5580397357678457   F   F   F
  7.4693821404696461  5.1844866945570187 12.3205669558782276   F   F   F
  7.3796063809232075  0.8284841653860766 12.2001224306209899   F   F   F
  3.4041526148381629  3.1417886655575238 13.7571037336873516   F   F   F
  7.3984920730023314  1.1740067621729322 15.0867947279535155   T   T   T
  3.3959153739962940  2.9203359255923207 16.4140651303244098   T   T   T
  4.8326707461918161  0.8284059606859262 12.2001609218852352   F   F   F
  0.6635062671094486  3.1418675584516125 13.7573467757868890   F   F   F
  4.8150109991080869  1.1697919743979928 15.0901449951868649   T   T   T
  0.6750893170034153  2.9251696524068920 16.3977652054041840   T   T   T
  0.7614284176533394  7.2750721063201693 16.4948840555701821   T   T   T
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4.7251586212103875	4.9742648496420436	14.9582450879265600	T	T	T
0.7593006500606559	6.9574738703598040	13.5580209908492506	F	F	F
4.7428648506031594	5.1844008270909452	12.3204488991888077	F	F	F
6.1175590598863403	7.0972979907859060	16.4222707196392150	T	T	T
6.1060957965632854	7.2415462809879134	13.5907646217275762	F	F	F
2.0338223799108510	1.0040686240886074	12.2256103096605884	F	F	F
2.0316500590717683	0.8872424598082669	15.0938086259832644	T	T	T
2.0355714900731945	5.1983877145180468	14.9866894983559948	T	T	T
2.0339049618479406	5.1108684680946661	12.3122395822918378	F	F	F
6.1062287607736385	2.9276630436989151	13.7206604568794788	F	F	F
6.1008115422055189	2.9890719075271597	16.4056096715516304	T	T	T
0.6115822782911097	4.9928077319819257	13.6140349333837065	F	F	F
4.7120022670648511	7.0245829671921678	12.2234202596149437	F	F	F
4.6893597707345611	3.1431420848132352	15.0995612847383036	T	T	T
0.6396602191601937	1.0808357123167893	16.4367226161552331	T	T	T
7.5247585911625148	3.1439466821580186	15.1013315876084508	T	T	T
3.4365499823993755	1.0736442209656445	16.4302730133423580	T	T	T
3.4557887564234040	4.9927315740952523	13.6140049494892601	F	F	F
7.5003821740159413	7.0246414996324837	12.2233730105456431	F	F	F
6.1059836221283641	1.0214609430191108	13.6748354828937444	F	F	F
6.1117724844857291	0.9719714095359254	16.3816687087493804	T	T	T
6.1059552502899548	6.0543509027547300	14.9843174671425245	T	T	T
2.0314480439939784	7.0918156343225034	15.0601264271535662	T	T	T
2.0337538904369699	7.1196392399368236	12.2590327337071869	F	F	F
2.0338786223286012	2.0687523053110657	13.6963480075419035	F	F	F
2.0345488444150446	4.0527071323216379	16.4076594744186011	T	T	T
6.1061211962709887	4.0785695544443232	12.2955930440659955	F	F	F
3.3921287463284209	6.9246432771534323	19.0064989831414870	T	T	T
7.4071533284550730	5.0072120687645088	18.0228009893584229	T	T	T
7.4217741218039750	0.8376557613991011	17.6560297070398136	T	T	T
3.3790433098108168	3.4167067017741086	19.5476814905917173	T	T	T
4.8191879960252733	0.8541803193718379	17.6817699589797606	T	T	T
0.7423085144560829	3.0648595024280367	19.5274190400741503	T	T	T
0.6674698866503178	6.8096524614213019	19.0402036159944821	T	T	T
4.7861347626264603	5.1025681818217308	17.9466549048099075	T	T	T
6.0689469222337546	7.2559437734960541	18.9740330889011695	T	T	T
2.0297973079223470	0.9998402437086664	17.7785492496810527	T	T	T
2.0261564380545614	4.9903872288743889	17.9405340798350572	T	T	T
6.0622295562696893	2.7182730373389741	19.3793341264082599	T	T	T
0.6005481187425632	4.9138493086216712	19.1707278559379724	T	T	T
4.7391999232273418	6.9838696936620535	17.7597469006771043	T	T	T
3.4910449099331058	5.1296905373033246	19.1467827207288721	T	T	T
7.4542148266597161	6.8876435601717692	17.8119732502907731	T	T	T
6.2236830845983198	0.9415034951155784	19.0459099650048636	T	T	T
2.0095725211638178	7.1811079186296300	17.9172143029592590	T	T	T
2.2068921219985516	2.1200919036479666	19.1505598579521141	T	T	T
6.0540867693826312	3.8877963859296387	17.9908855628402016	T	T	T
3.2704341331597999	1.2203671524451307	20.2736900436830325	T	T	T
7.4680920456306827	0.6223648054710077	20.3931859375321629	T	T	T
0.7127347009499958	0.0410239885525728	21.6520343257322523	T	T	T
2.0122999150583185	1.4465811604692655	23.4807948028055868	T	T	T
0.6570422299199845	0.0898611865666825	25.4543105359407811	T	T	T
0.6466722570348605	2.8682145322332051	21.6060819907629451	T	T	T
2.0139041732828593	4.1170205527858110	23.5295492919570499	T	T	T
0.6587142208551068	2.7795391376530558	25.4455940503350213	T	T	T
0.6658758149110809	5.4953155299315881	21.7224058846467400	T	T	T
2.0038758418722580	6.8919984415095010	23.5608778165101960	T	T	T
0.6600014247866854	5.4959536497994392	25.4632498602401931	T	T	T
3.3640345123318958	-0.1079451726060222	21.6791864155736924	T	T	T
4.7398492374311783	1.4489015565823467	23.4854410193655738	T	T	T
3.3822993463051807	0.0884045674391573	25.4474530938207657	T	T	T
3.4137322047108150	2.8683408846261500	21.5633000214694768	T	T	T
4.7514153158627739	4.1224344467268184	23.5196606657026805	T	T	T

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  3.3786338805940597  2.7865075301997235 25.4432067642131443   T   T   T
  3.3753348198691855  5.4932276713466850 21.7690777546439733   T   T   T
  4.7508919363927875  6.8761718017743592 23.5542687892267466   T   T   T
  3.3789384383546119  5.4775187181338687 25.4810515847515688   T   T   T
  6.0242939602403567  0.0674427104113425 21.6782889525719149   T   T   T
  7.4517836994137641  1.4567355988466946 23.4800767390768179   T   T   T
  6.0916885521492539  0.0791956682665148 25.4640382985869280   T   T   T
  6.0771387838470705  2.9026204515072682 21.5345761367463702   T   T   T
  7.4310524186961961  4.1387270211865985 23.5066367948980286   T   T   T
  6.0915807456603144  2.7754831127791979 25.4435401016071587   T   T   T
  6.0868124790343758  5.5321992091347161 21.6902297801285258   T   T   T
  7.4479822203578969  6.8550720144677735 23.5671165763956765   T   T   T
  6.1021683189867684  5.4957407307127344 25.4709939617943135   T   T   T
  2.0227522296703060  1.4359576978178528 27.4019895396653403   T   T   T
  0.6625958664747876  0.0684782114558035 29.2293848784878136   T   T   T
  2.0174098319125227  4.1415786388304596 27.3985690612906474   T   T   T
  0.6647554352013217  2.7874137168335604 29.2357835473571619   T   T   T
  2.0277373711860789  6.8656622549279316 27.3916839850164457   T   T   T
  0.6618947316952980  5.5016337991086832 29.2278456492585796   T   T   T
  4.7326773316922877  1.4292447832502657 27.4008086543901861   T   T   T
  3.3770041404542313  0.0672590386936129 29.2258173326513102   T   T   T
  4.7396735849883553  4.1388845717866545 27.3993713563234387   T   T   T
  3.3789978514338923  2.7840606867153941 29.2369259135679052   T   T   T
  4.7322751846278228  6.8560424594349607 27.3988584712873084   T   T   T
  3.3772766335464222  5.4993475274862265 29.2285298737447725   T   T   T
  7.4496480023621823  1.4284254470165088 27.4023283219800184   T   T   T
  6.0935426375541795  0.0717301633555380 29.2332757697881824   T   T   T
  7.4523999187575294  4.1292292542461144 27.3985523808349036   T   T   T
  6.0913710844700919  2.7862351026688512 29.2377038897032868   T   T   T
  7.4516148911383286  6.8598278505343906 27.4010347906033793   T   T   T
  6.0957314575498334  5.4998220607877144 29.2300082621677042   T   T   T

Oxide reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Ir E_tot= -694.34530974 eV
 D3-zero damping= -11.088345 eV, D3-BJ damping= -16.667928 eV
 O Al  O Al  O Al  H  O  H  O  H
 1.0000000000000000
     8.1451896436500029    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1451896436500029    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6840463963622163
  18  12  24  16  12   8   1   1   1   1   2
Selective dynamics
Cartesian
  3.3072904583944931  7.3116908143261332 10.9423958550990683   F   F   F
  7.4763745023913755  4.9983163188278228  9.3854545373318210   F   F   F
  3.3082910715743270  6.9577252432591177  8.0000187449185951   F   F   F
  3.4041526148381629  3.1417886655575238  8.1990827428381010   F   F   F
  7.3808727607516316  1.1824204517855503  9.5845317789161726   F   F   F
  3.3973198105747153  2.9554827856932442 10.8220669229527680   F   F   F
  0.6635062671094486  3.1418675584516125  8.1993257849376384   F   F   F
  4.8319300655521626  1.1823186423485719  9.5846030099037201   F   F   F
  0.6707128935075548  2.9553588206858872 10.8217845066302907   F   F   F
  0.7603964561024460  7.3117963931275423 10.9423584978630899   F   F   F
  4.7356112412567306  4.9984034152108698  9.3853700880230981   F   F   F
  0.7593006500606559  6.9574738703598040  8.0000000000000000   F   F   F
  6.1061383560451192  7.1360127545775418 10.9172067463060003   F   F   F
  6.1060957965632854  7.2415462809879134  8.0327436308783255   F   F   F
  2.0341472910358536  0.8984737569744050  9.5519775531218265   F   F   F
  2.0340365696148570  5.2123499945203990  9.4220834377914784   F   F   F
  6.1062287607736385  2.9276630436989151  8.1626394660302282   F   F   F
  6.1063098410967482  3.0291140098502445 10.8301543211852653   F   F   F
  0.6115822782911097  4.9928077319819257  8.0560139425344559   F   F   F
  4.6842048365635867  3.1474342666135295  9.5285274732362595   F   F   F
  0.6395664378216807  1.1153311483044748 10.9191009939757393   F   F   F
```

7.5283923640208785	3.1473813565250790	9.5284873332419124	F	F	F
3.4279967790872825	1.1153911737965609	10.9192047381793635	F	F	F
3.4557887564234040	4.9927315740952523	8.0559839586400095	F	F	F
6.1059836221283641	1.0214609430191108	8.1168144920444938	F	F	F
6.1063447748432020	1.0206483839901006	10.8835529458276739	F	F	F
6.1060501375520069	6.0713976433900552	9.4463612987341463	F	F	F
2.0342164981411819	7.1185924067110227	9.4677862360962415	F	F	F
2.0338786223286012	2.0687523053110657	8.1383270166926529	F	F	F
2.0339878610329807	4.0613397090583305	10.8469192662674665	F	F	F
3.2978930698010851	7.3363623926659258	16.5870951940545588	T	T	T
7.4822561886816210	4.9734849998920545	14.9595850915972619	T	T	T
3.3082910715743270	6.9577252432591177	13.5580397357678457	F	F	F
7.4693821404696461	5.1844866945570187	12.3205669558782276	F	F	F
7.3796063809232075	0.8284841653860766	12.2001224306209899	F	F	F
3.4041526148381629	3.1417886655575238	13.7571037336873516	F	F	F
7.4075532404011346	1.1569343747386986	15.1046491127694136	T	T	T
3.4121103533026469	2.9362843807489680	16.3871229101262621	T	T	T
4.8326707461918161	0.8284059606859262	12.2001609218852352	F	F	F
0.6635062671094486	3.1418675584516125	13.7573467757868890	F	F	F
4.8096757390490490	1.1607404967341572	15.1002359248162286	T	T	T
0.6403802425297678	2.9365402628545199	16.4033433288031567	T	T	T
0.7940730817011247	7.3317547053816643	16.5939515277345038	T	T	T
4.7287276755753993	4.9769643172318263	14.9605707878544667	T	T	T
0.7593006500606559	6.9574738703598040	13.5580209908492506	F	F	F
4.7428648506031594	5.1844008270909452	12.3204488991888077	F	F	F
6.0988024667370473	7.1315955579227390	16.4544876003614355	T	T	T
6.1060957965632854	7.2415462809879134	13.5907646217275762	F	F	F
2.0338223799108510	1.0040686240886074	12.2256103096605884	F	F	F
2.0308606226017591	0.9042778992733587	15.1367250270245908	T	T	T
2.0319888829137431	5.2159793387759708	14.9776188789872720	T	T	T
2.0339049618479406	5.1108684680946661	12.3122395822918378	F	F	F
6.1062287607736385	2.9276630436989151	13.7206604568794788	F	F	F
6.1078693274199773	2.9705003721952963	16.3339494514075660	T	T	T
0.6115822782911097	4.9928077319819257	13.6140349333837065	F	F	F
4.7120022670648511	7.0245829671921678	12.2234202596149437	F	F	F
4.6933822513950991	3.1298823551926183	15.0679236308021558	T	T	T
0.6440914882888742	1.1090239722495592	16.5132601365496683	T	T	T
7.5196595817980816	3.1245605455793179	15.0636968794606521	T	T	T
3.4123644992197004	1.1149411393374891	16.4856917813987032	T	T	T
3.4557887564234040	4.9927315740952523	13.6140049494892601	F	F	F
7.5003821740159413	7.0246414996324837	12.2233730105456431	F	F	F
6.1059836221283641	1.0214609430191108	13.6748354828937444	F	F	F
6.1093874560323211	0.9494336796798011	16.3837462920191932	T	T	T
6.1070336792388460	6.0711951726002544	14.9993661995363254	T	T	T
2.0308943478828532	7.1107317304273128	15.0998702414883734	T	T	T
2.0337538904369699	7.1196392399368236	12.2590327337071869	F	F	F
2.0338786223286012	2.0687523053110657	13.6963480075419035	F	F	F
2.0288185522987869	4.0113188985701758	16.3183409679474032	T	T	T
6.1061211962709887	4.0785695544443232	12.2955930440659955	F	F	F
3.4158606250680910	6.7014070789295976	19.1157402822635873	T	T	T
7.4192596494625480	5.1495812292297796	17.8598430611834296	T	T	T
7.4011474519315348	0.8412376234358481	17.7290201242613890	T	T	T
3.3833919200251956	3.3574453076921058	19.7222998273299837	T	T	T
4.7893505689810052	0.9062779287152952	17.6970230578108776	T	T	T
0.6337214030492202	3.3700007588004808	19.6623447838395435	T	T	T
0.7043203168200940	6.7535588740727750	19.1519425930331515	T	T	T
4.8543780456682430	5.0748750784676666	17.8673256481748979	T	T	T
6.0998284960200673	7.3517915360386539	19.0714514951814600	T	T	T
2.0253098585335065	1.0978182898635729	17.9288074210128769	T	T	T
2.0574635397203020	4.9295953212622923	17.8292879689837065	T	T	T
6.4066263802236518	2.8036764029442645	19.1773930534181645	T	T	T
0.6318348532146998	4.9523151448742855	18.9133622789762086	T	T	T
4.7634501355631302	6.9543177540384544	17.8382659269846684	T	T	T

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  3.4982084218666420  4.8866966186700234 18.9223361729559549   T   T   T
  7.4723058437174572  7.0298719656523785 17.8711961468261826   T   T   T
  5.9569919300500533  1.0111511135422226 19.0833220458080000   T   T   T
  2.0587593315228405  7.3029957887051946 18.0611282123231121   T   T   T
  2.0126186568487565  2.2352808240484592 19.5045481939421101   T   T   T
  6.1673301926038047  3.9431145287436333 17.8033760314771072   T   T   T
  7.4207192604331329  2.9676643949207504 19.4881974436672571   T   T   T
  2.2015640748082990  0.9966476601859594 20.7287239219702606   T   T   T
  1.7210070739296042  0.1531608750184605 20.6679876222655601   T   T   T
  4.8456662943321893  1.3154087419620868 20.5617940881640351   T   T   T
  4.4725970170990630  2.2555676293821416 20.4236229502410396   T   T   T
  3.9951050795245937  0.7970449007399567 20.7171474735106678   T   T   T

Metal reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Ir E_tot= -398.20657225 eV
 D3-zero damping= -23.8108995 eV, D3-BJ damping= -25.0242167 eV
Ir
 1.0000000000000000
     8.1451896436500029    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1451896436500029    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0002798442392654 -0.0002800191392171  8.0568916680494471
  1.3571590845927890  1.3571588741174361  9.8876191036087384
 -0.0004570447348009 -0.0004570792896131 11.8276015897431694
  1.3567566149253463  1.3567566950342165 13.7678490544673018
 -0.0007900565755808 -0.0007899466945541 15.5987926047195593
 -0.0002447812562515  2.7147740414621095  8.0569498530224415
  1.3571773460458718  4.0722852325851413  9.8874382930875395
 -0.0005077959345058  2.7145956018077748 11.8276045481942305
  1.3568613442787136  4.0719230501926766 13.7679664692265629
 -0.0006574622226124  2.7143669859322759 15.5985915135074116
 -0.0002492176801693  5.4299021328385777  8.0569530400386764
  1.3571523202601914  6.7874010974721539  9.8876170503683269
 -0.0004558803362309  5.4296442635444535 11.8275931755308665
  1.3567376737905583  6.7870777241239129 13.7678076910423357
 -0.0007125651108604  5.4294527739395564 15.5985739600482276
  2.7147741916988752 -0.0002449183364295  8.0569499721699653
  4.0722853195967614  1.3571770949336159  9.8874382940801127
  2.7145955558505817 -0.0005077899224245 11.8276045431862382
  4.0719228018809090  1.3568613940624581 13.7679664675800293
  2.7143668063372686 -0.0006573716379037 15.5985914384189535
  2.7148113971455019  2.7148111992662107  8.0567322342520811
  4.0722692999470009  4.0722691822375356  9.8872815348782179
  2.7147368722918559  2.7147368919566386 11.8276880311105366
  4.0719974933628835  4.0719977356538388 13.7680120065208023
  2.7144139561738374  2.7144141675377296 15.5988616156143980
  2.7148104483069764  5.4298735870089443  8.0567381312202802
  4.0722729116345207  6.7873279190569091  9.8874241432959273
  2.7146653960081664  5.4294899827352427 11.8277012333384199
  4.0719140696564100  6.7869936366617933 13.7679517320240219
  2.7143946899100384  5.4294822092805894 15.5988122176703783
  5.4299022925957718 -0.0002493437176963  8.0569529909489361
  6.7874012111253652  1.3571521190212568  9.8876170569754738
  5.4296441759375380 -0.0004559109540933 11.8275931440159088
  6.7870776273913380  1.3567376957423669 13.7678076724008047
  5.4294526067121742 -0.0007124623355347 15.5985739652085353
  5.4298737407453217  2.7148103015978364  8.0567380103415385
  6.7873281168755888  4.0722727728664161  9.8874241203196718
  5.4294899296723536  2.7146654085973214 11.8277012392916063
  6.7869935307697284  4.0719142616346451 13.7679517147750943
  5.4294820443910066  2.7143949456707785 15.5988122511544454
  5.4298794157802135  5.4298791899920724  8.0567296777420641
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  6.7874025853856468  6.7874023679117830  9.8876198588143431
  5.4295140362835497  5.4295140352521711 11.8276428900953263
  6.7870469000109042  6.7870470153464648 13.7677651371691852
  5.4294266363748367  5.4294267474240847 15.5988587611836493

Interface: 2O-g-Al2O3(110)/fcc(100)_3x3/Rh E_tot= -1008.83942814 eV
 D3-zero damping= -34.5936345 eV, D3-BJ damping= -43.1032224 eV
 O Al  O Al  O Al  O Rh
 1.0000000000000000
     8.0329880858400013    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.0329880858400013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.2716937760818396
  18  12  24  16  12   8   2  45
Selective dynamics
Cartesian
  3.2617318946535843  7.2109708635964349 10.9423958550990683   F   F   F
  7.3733860021060238  4.9294635478138478  9.3854545373318210   F   F   F
  3.2627187241939386  6.8618812365187392  8.0000187449185951   F   F   F
  3.3572597562163131  3.0985099209232376  8.1990827428381010   F   F   F
  7.2791998153709958  1.1661323820804854  9.5845317789161726   F   F   F
  3.3505210751490235  2.9147704404756039 10.8220669229527680   F   F   F
  0.6543663403498037  3.0985877270524989  8.1993257849376384   F   F   F
  4.7653692972578847  1.1660319750881312  9.5846030099037201   F   F   F
  0.6614736940797710  2.9146481831101250 10.8217845066302907   F   F   F
  0.7499218483080882  7.2110749880294982 10.9423584978630899   F   F   F
  4.6703772833382917  4.9295494444274253  9.3853700880230981   F   F   F
  0.7488411372058054  6.8616333263295806  8.0000000000000000   F   F   F
  6.0220251228700281  7.0377128029932523 10.9172067463060003   F   F   F
  6.0219831496532619  7.1417925847294708  8.0327436308783255   F   F   F
  2.0061265198992171  0.8860971077379413  9.5519775531218265   F   F   F
  2.0060173236871433  5.1405488683560643  9.4220834377914784   F   F   F
  6.0221142822559814  2.8873339207911530  8.1626394660302282   F   F   F
  6.0221942456820070  2.9873873803230535 10.8301543211852653   F   F   F
  0.6031576144888678  4.9240308428138597  8.0560139425344559   F   F   F
  4.6196790117814324  3.1040777527361723  9.5285274732362595   F   F   F
  0.6307562868262977  1.0999672466903065 10.9191009939757393   F   F   F
  7.4246873076620501  3.1040255714943914  9.5284873332419124   F   F   F
  3.3807754625055231  1.1000264453196658 10.9192047381793635   F   F   F
  3.4081845999952867  4.9239557340167588  8.0559839586400095   F   F   F
  6.0218725204428107  1.0073901215818017  8.1168144920444938   F   F   F
  6.0222286982093678  1.0065887557100852 10.8835529458276739   F   F   F
  6.0219381196036679  5.9877629702301212  9.4463612987341463   F   F   F
  2.0061947736633257  7.0205324237774009  9.4677862360962415   F   F   F
  2.0058615521552090  2.0402548434306178  8.1383270166926529   F   F   F
  2.0059692860753731  4.0053939715017819 10.8469192662674665   F   F   F
  3.2604877902048148  7.1630570705106500 16.5624413548946130   T   T   T
  7.3894154866975263  4.9263075624535499 14.9728357295997014   T   T   T
  3.2627187241939386  6.8618812365187392 13.5580397357678457   F   F   F
  7.3664899613179591  5.1130693907219849 12.3205669558782276   F   F   F
  7.2779508801688779  0.8170716362683897 12.2001224306209899   F   F   F
  3.3572597562163131  3.0985099209232376 13.7571037336873516   F   F   F
  7.3032545932123947  1.1390310526255880 15.1014332861114742   T   T   T
  3.3539390073018542  2.9029256115588851 16.4258134306606003   T   T   T
  4.7660997748789171  0.8169945088530625 12.2001609218852352   F   F   F
  0.6543663403498037  3.0985877270524989 13.7573467757868890   F   F   F
  4.7340924075608122  1.1370256696172070 15.1089209609599742   T   T   T
  0.6632658664424911  2.8986526138607780 16.4141961297874452   T   T   T
  0.7425926165117772  7.1544947054547725 16.5362529767539321   T   T   T
  4.6540159587852425  4.9241962812403948 14.9736865231928622   T   T   T
  0.7488411372058054  6.8616333263295806 13.5580209908492506   F   F   F
  4.6775309728174106  5.1129847060968121 12.3204488991888077   F   F   F
  6.0163242990421262  7.0194122543593398 16.4864459301394461   T   T   T
  6.0219831496532619  7.1417925847294708 13.5907646217275762   F   F   F
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2.0058060844876073	0.9902373851979678	12.2256103096605884	F	F	F
2.0111206934311538	0.8649066605442498	15.1047259653047199	T	T	T
2.0079627734201448	5.1268908278190901	15.0013737463064292	T	T	T
2.0058875288425910	5.0404652695234331	12.3122395822918378	F	F	F
6.0221142822559814	2.8873339207911530	13.7206604568794788	F	F	F
6.0190499182937556	2.9560905118458036	16.3925521627594861	T	T	T
0.6031576144888678	4.9240308428138597	13.6140349333837065	F	F	F
4.6470935273179368	6.9278179824138180	12.2234202596149437	F	F	F
4.6177953589625087	3.1035532984760619	15.1018680013537612	T	T	T
0.6378674547004947	1.0592611776493408	16.4330979189765891	T	T	T
7.4235848795570831	3.1075756883271843	15.1043192374297934	T	T	T
3.3809349261438135	1.0670914187118283	16.4679436283966645	T	T	T
3.4081845999952867	4.9239557340167588	13.6140049494892601	F	F	F
7.3970629634250580	6.9278757085584823	12.2233730105456431	F	F	F
6.0218725204428107	1.0073901215818017	13.6748354828937444	F	F	F
6.0176698257049663	0.9575523037629958	16.3980870992945142	T	T	T
6.0206879815003580	6.0050833481523940	15.0186787323922033	T	T	T
2.0071938572406038	6.9878921250946826	15.0840144454488154	T	T	T
2.0057385384694340	7.0215648366736776	12.2590327337071869	F	F	F
2.0058615521552090	2.0402548434306178	13.6963480075419035	F	F	F
2.0063143449181240	4.0330562329570085	16.4469002119051879	T	T	T
6.0220081994750956	4.0223864724455067	12.2955930440659955	F	F	F
3.3424456786522678	6.8096112214177724	19.1774353069966210	T	T	T
7.3015187290120886	5.0254317677620515	17.9863397965877780	T	T	T
7.3302654576122368	0.8479510306050665	17.6867933658063841	T	T	T
3.3150251984202108	3.1204354117226680	19.5237831870838221	T	T	T
4.7378999833568889	0.8515513545554242	17.7259183697613025	T	T	T
0.6028505061541266	3.0987279393972247	19.4822070831571068	T	T	T
0.6300379721407771	6.7836643226658913	19.1382247180933405	T	T	T
4.6884339656316456	5.0592091295456409	17.9925596121805498	T	T	T
5.9993929816592484	7.2398978230700353	19.1019144259301399	T	T	T
1.9959043308268420	0.9732551255918748	17.7666234810075139	T	T	T
1.9956629546214202	4.9703734618915432	17.9911405156844602	T	T	T
5.8998601464988392	2.7794696403872776	19.3007268768840419	T	T	T
0.5388069217449799	4.8837378734984123	19.2078138952808359	T	T	T
4.6637072089890959	6.9056793506996508	17.8710023014857171	T	T	T
3.4370498303248214	4.8947079211480240	19.2265743752937048	T	T	T
7.3549477916493000	6.8645694167580498	17.8487695474766142	T	T	T
6.1299264581324318	1.0442327145211119	19.0477076078890590	T	T	T
1.9881270154046189	7.0495143951261863	17.9855595276243143	T	T	T
1.9717409319783727	2.0663060421071799	19.1473419268698208	T	T	T
5.9778212884772675	3.8847933202864557	17.9442194820662877	T	T	T
2.0858170286816224	0.9196002892873393	20.5080234108661514	T	T	T
7.1760315012672633	1.0004599803283891	20.5910916987309314	T	T	T
0.5902787320443086	-0.2188846902644996	21.5122020642176928	T	T	T
1.8808306745978609	1.1595621402504581	23.4551767758889547	T	T	T
0.5303649925399292	-0.1703542191636588	25.3494237985379911	T	T	T
0.4510939118045225	2.6381719838850621	21.5629010668400802	T	T	T
1.8560445520238458	3.8108267457768257	23.4801505995521076	T	T	T
0.5276309509047409	2.4841647874975950	25.3459257210908220	T	T	T
0.5441317820474297	5.1891215977511793	21.7214991338094698	T	T	T
1.8831801860389985	6.5507630924079665	23.4704867323135815	T	T	T
0.5416290207336597	5.1844340534929589	25.3611279253965201	T	T	T
3.3490243844404533	-0.3592810944421927	21.4135122990747284	T	T	T
4.5472828384333983	1.1268945888163229	23.3956993558001294	T	T	T
3.2225148653166493	-0.1842900359726768	25.3471899997014916	T	T	T
3.2366227280538711	2.5058101639672024	21.5637186869120576	T	T	T
4.5683125945827383	3.7907922867918060	23.4399741882470636	T	T	T
3.2166257405419936	2.4800249758058821	25.3330489117723019	T	T	T
3.2117652716943828	5.1413506208966009	21.7185932817558296	T	T	T
4.5711354394480104	6.5256296044494455	23.4529471788951192	T	T	T
3.2226415233099730	5.1550959371726606	25.3641695906470446	T	T	T
5.8852370796113256	-0.2803843907048097	21.5213477752842799	T	T	T

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  7.2307488511219029  1.1760990264291300 23.4665514610652082   T   T   T
  5.8879564585784721 -0.1883217986087834 25.3529773427441079   T   T   T
  5.8651353169340696  2.5875664267910392 21.4625971487857257   T   T   T
  7.2033690287808243  3.8500624879414427 23.4895345954127883   T   T   T
  5.8814648861861993  2.4752644452167725 25.3424786154248736   T   T   T
  5.8898599360140143  5.1633330144558967 21.6338812735459030   T   T   T
  7.2412181684145782  6.5341171751517786 23.4755823601708045   T   T   T
  5.8829202410700745  5.1625486394678672 25.3808868207838039   T   T   T
  1.8717930785382788  1.1588550869588468 27.2738517213706437   T   T   T
  0.5359588751291798 -0.1998609421935978 29.0932755783754189   T   T   T
  1.8735664790207935  3.8234865682910661 27.2556463531508690   T   T   T
  0.5355258879688553  2.5033830450018590 29.0932550234094798   T   T   T
  1.8773377492359691  6.5181131394050675 27.2444389967626144   T   T   T
  0.5357873943202588  5.1731379467918641 29.0878813909109759   T   T   T
  4.5529023406168401  1.1560916640651981 27.2657893688060398   T   T   T
  3.2102765964025863 -0.1912010167501680 29.0957035566962112   T   T   T
  4.5517056213842855  3.8199175652594981 27.2615930341163484   T   T   T
  3.2170319263161864  2.4971410149141993 29.0975147509408032   T   T   T
  4.5489418034240767  6.5102441497129799 27.2560353856335844   T   T   T
  3.2119126696805176  5.1764482222230042 29.0905338103161561   T   T   T
  7.2242348856336704  1.1478507480173881 27.2750890255779836   T   T   T
  5.8835076380176901 -0.1970413302178241 29.0993315234265388   T   T   T
  7.2333717075138546  3.8174649425910498 27.2541068948711249   T   T   T
  5.8872304583578199  2.4930052063858543 29.1005333258323944   T   T   T
  7.2282123140912162  6.5065456812613336 27.2657997959404739   T   T   T
  5.8884921685966525  5.1683396703032365 29.0977297205378420   T   T   T

Oxide reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Rh E_tot= -693.47706457 eV
 D3-zero damping= -11.3736234 eV, D3-BJ damping= -17.0814758 eV
 O Al  O Al  O Al  H  O  H  O  H
 1.0000000000000000
     8.0329880858400013    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.0329880858400013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6840463963622163
  18  12  24  16  12   8   1   1   1   1   2
Selective dynamics
Cartesian
  3.2617318946535843  7.2109708635964349 10.9423958550990683   F   F   F
  7.3733860021060238  4.9294635478138478  9.3854545373318210   F   F   F
  3.2627187241939386  6.8618812365187392  8.0000187449185951   F   F   F
  3.3572597562163131  3.0985099209232376  8.1990827428381010   F   F   F
  7.2791998153709958  1.1661323820804854  9.5845317789161726   F   F   F
  3.3505210751490235  2.9147704404756039 10.8220669229527680   F   F   F
  0.6543663403498037  3.0985877270524989  8.1993257849376384   F   F   F
  4.7653692972578847  1.1660319750881312  9.5846030099037201   F   F   F
  0.6614736940797710  2.9146481831101250 10.8217845066302907   F   F   F
  0.7499218483080882  7.2110749880294982 10.9423584978630899   F   F   F
  4.6703772833382917  4.9295494444274253  9.3853700880230981   F   F   F
  0.7488411372058054  6.8616333263295806  8.0000000000000000   F   F   F
  6.0220251228700281  7.0377128029932523 10.9172067463060003   F   F   F
  6.0219831496532619  7.1417925847294708  8.0327436308783255   F   F   F
  2.0061265198992171  0.8860971077379413  9.5519775531218265   F   F   F
  2.0060173236871433  5.1405488683560643  9.4220834377914784   F   F   F
  6.0221142822559814  2.8873339207911530  8.1626394660302282   F   F   F
  6.0221942456820070  2.9873873803230535 10.8301543211852653   F   F   F
  0.6031576144888678  4.9240308428138597  8.0560139425344559   F   F   F
  4.6196790117814324  3.1040777527361723  9.5285274732362595   F   F   F
  0.6307562868262977  1.0999672466903065 10.9191009939757393   F   F   F
  7.4246873076620501  3.1040255714943914  9.5284873332419124   F   F   F
  3.3807754625055231  1.1000264453196658 10.9192047381793635   F   F   F
  3.4081845999952867  4.9239557340167588  8.0559839586400095   F   F   F
  6.0218725204428107  1.0073901215818017  8.1168144920444938   F   F   F
  6.0222286982093678  1.0065887557100852 10.8835529458276739   F   F   F
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6.0219381196036679	5.9877629702301212	9.4463612987341463	F	F	F
2.0061947736633257	7.0205324237774009	9.4677862360962415	F	F	F
2.0058615521552090	2.0402548434306178	8.1383270166926529	F	F	F
2.0059692860753731	4.0053939715017819	10.8469192662674665	F	F	F
3.2573052825761164	7.2175169046636336	16.6161137408479647	T	T	T
7.3874757718732864	4.9158472697392250	14.9724717954881470	T	T	T
3.2627187241939386	6.8618812365187392	13.5580397357678457	F	F	F
7.3664899613179591	5.1130693907219849	12.3205669558782276	F	F	F
7.2779508801688779	0.8170716362683897	12.2001224306209899	F	F	F
3.3572597562163131	3.0985099209232376	13.7571037336873516	F	F	F
7.3164102438186251	1.1272832494301537	15.1187054372630882	T	T	T
3.3680708060280375	2.9104524941489078	16.4099107967589006	T	T	T
4.7660997748789171	0.8169945088530625	12.2001609218852352	F	F	F
0.6543663403498037	3.0985877270524989	13.7573467757868890	F	F	F
4.7326628864490781	1.1309008815277648	15.1147044617437984	T	T	T
0.6275253555479584	2.9115170794686676	16.4282553647616787	T	T	T
0.7799667159726624	7.2151272913779092	16.6249194372561249	T	T	T
4.6558111842664491	4.9199655832203231	14.9732755159613991	T	T	T
0.7488411372058054	6.8616333263295806	13.5580209908492506	F	F	F
4.6775309728174106	5.1129847060968121	12.3204488991888077	F	F	F
6.0176919177122228	7.0340218918728654	16.4818762304514763	T	T	T
6.0219831496532619	7.1417925847294708	13.5907646217275762	F	F	F
2.0058060844876073	0.9902373851979678	12.2256103096605884	F	F	F
2.0029566891948609	0.8928811987863206	15.1555373529845046	T	T	T
2.0039905284167836	5.1459424596889241	14.9945272288295328	T	T	T
2.0058875288425910	5.0404652695234331	12.3122395822918378	F	F	F
6.0221142822559814	2.8873339207911530	13.7206604568794788	F	F	F
6.0243359465410595	2.9258047259544719	16.3455396556401844	T	T	T
0.6031576144888678	4.9240308428138597	13.6140349333837065	F	F	F
4.6470935273179368	6.9278179824138180	12.2234202596149437	F	F	F
4.6229783682116468	3.0883842121174365	15.0800892064633683	T	T	T
0.6379005731886106	1.0968151480154826	16.5421366783977390	T	T	T
7.4218580353754628	3.0819689725150012	15.0753030199112210	T	T	T
3.3630889815182483	1.1019471121179767	16.5138605658880842	T	T	T
3.4081845999952867	4.9239557340167588	13.6140049494892601	F	F	F
7.3970629634250580	6.9278757085584823	12.2233730105456431	F	F	F
6.0218725204428107	1.0073901215818017	13.6748354828937444	F	F	F
6.0254613415807219	0.9395267741477560	16.4054679618403405	T	T	T
6.0235356662742312	6.0066141628322907	15.0156250988584805	T	T	T
2.0030582904197289	7.0141849104637002	15.1110940508925520	T	T	T
2.0057385384694340	7.0215648366736776	12.2590327337071869	F	F	F
2.0058615521552090	2.0402548434306178	13.6963480075419035	F	F	F
2.0006579462161298	3.9916347588616268	16.3665873772072210	T	T	T
6.0220081994750956	4.0223864724455067	12.2955930440659955	F	F	F
3.3811186580302555	6.6264042817295499	19.1765866067716892	T	T	T
7.3331617644028881	5.0674325459295897	17.8849515153792460	T	T	T
7.3013302302764886	0.8447836873292518	17.7622358590092091	T	T	T
3.3370258988655874	3.3019262407724406	19.8135049311936093	T	T	T
4.7188009967026021	0.9009008638338869	17.7339237670076102	T	T	T
0.6066260770007342	3.3158160409239890	19.7473850546410752	T	T	T
0.6882215054083707	6.6823709002379745	19.2136462635996850	T	T	T
4.7739610128672876	4.9899583077434873	17.8911576282948310	T	T	T
6.0204554472479872	7.2296666176916951	19.1090620661466524	T	T	T
1.9987193725482730	1.0872652522790844	17.9672115167077955	T	T	T
2.0307211484268373	4.8713673604906855	17.8981792547807714	T	T	T
6.2966498358800358	2.7717733773442483	19.2302213897238445	T	T	T
0.6133804215071624	4.8889152615087532	18.9920332534376186	T	T	T
4.6970537781065405	6.8537166542258072	17.8647518802415348	T	T	T
3.4649731969915818	4.8177192982335253	19.0024313047693383	T	T	T
7.3735641428692382	6.9316273028644666	17.8984136018506916	T	T	T
5.8695422472244969	0.9901837472103366	19.1306190348527636	T	T	T
2.0334336202075818	7.1876303686156096	18.0954147887505457	T	T	T
1.9776929458139523	2.1757021981785885	19.5696852730589903	T	T	T

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  6.0854390529976490  3.8677377039738179 17.8267289836728935   T   T   T
  7.3154726146997309  2.9346893837013024 19.5595801332419725   T   T   T
  2.1362896834916865  0.9287011358655689 20.7847964851238416   T   T   T
  1.6651708777448064  0.0830483205533443 20.6790338858036193   T   T   T
  4.7865413128919450  1.2551974040751932 20.6376568883072196   T   T   T
  4.4162361132424843  2.1981424330753057 20.5216491056056256   T   T   T
  3.9378210882586573  0.7304469501985836 20.7812924147619071   T   T   T

Metal reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Rh E_tot= -327.12330447 eV
 D3-zero damping= -19.3210663 eV, D3-BJ damping= -22.4126897 eV
Rh
 1.0000000000000000
     8.0329880858400013    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.0329880858400013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0003155027487574 -0.0003133579117291  8.0889891459620102
  1.3384376326513099  1.3384348145679728  9.9206979029047417
 -0.0008827891331823 -0.0008721075381926 11.8276838387698184
  1.3381977302843577  1.3381892973316925 13.7354434410448221
 -0.0006629120124709 -0.0006653430154914 15.5664906175198148
 -0.0001827917914599  2.6772966337827211  8.0915786761431772
  1.3385323974649270  4.0159180678141553  9.9215091613356847
 -0.0004278480714868  2.6761657572115851 11.8278684661890452
  1.3381419333702242  4.0158083854955953 13.7343079870090357
 -0.0003845355450809  2.6770518128987950 15.5639950898660100
 -0.0002346758408553  5.3550103640989803  8.0915768074533538
  1.3382884564314419  6.6936492816352899  9.9202506299082991
 -0.0006174111265524  5.3550222982432585 11.8274410088403421
  1.3383385090992137  6.6930358014614244 13.7352239141672055
 -0.0005649400981955  5.3545502203519684 15.5637808782028202
  2.6773112541004394 -0.0000611861572501  8.0915860762173626
  4.0159302255602833  1.3385292031710490  9.9215011901375227
  2.6761504294973029 -0.0004843855502316 11.8278763389795696
  4.0158106158183093  1.3381294703497566 13.7342909772195103
  2.6770485662973624 -0.0003839734108014 15.5639974445102975
  2.6777192802994536  2.6777220264064590  8.0909390338675315
  4.0161489801522956  4.0161519492249225  9.9224563858999257
  2.6771031681837862  2.6770697464533004 11.8274728524137309
  4.0158852187421417  4.0158787935051938 13.7330191220469189
  2.6774358118276647  2.6774255670120919 15.5642436815892733
  2.6775840561348270  5.3548696572205063  8.0909809497277987
  4.0159225128538356  6.6941789222509671  9.9214783067905827
  2.6770689196694577  5.3551935152785326 11.8277164449983161
  4.0156832575488508  6.6942304620168551 13.7341352421476000
  2.6773731206987326  5.3547778135191804 15.5642196151160075
  5.3550205699767996 -0.0002258472658032  8.0915784266744240
  6.6936486610207355  1.3382985585550145  9.9202589850943230
  5.3550222543762773 -0.0006087393603481 11.8274411460925286
  6.6930444516733729  1.3383479137121488 13.7352182647289407
  5.3545537018615983 -0.0005630119294872 15.5637804660935046
  5.3548731279103761  2.6776387074344701  8.0909612769725197
  6.6941783072290368  4.0159262901463304  9.9214947331544341
  5.3552955253805727  2.6770855661686190 11.8277871014582328
  6.6942371248290460  4.0156788297494526 13.7341181476547760
  5.3547750695152034  2.6773717025023229 15.5642088718491785
  5.3549639099020068  5.3549854485767199  8.0909423341568694
  6.6937401069779456  6.6937461220132013  9.9198655657292267
  5.3550306678636685  5.3550292648649016 11.8275277490694979
  6.6932850409585880  6.6932850628581511 13.7353432442495436
  5.3548001485768433  5.3548013106047883 15.5641142017244736
```

```
Interface: 2O-g-Al2O3(110)/fcc(100)_3x3/Os E_tot= -1173.77300488 eV
 D3-zero damping= -33.8567813 eV, D3-BJ damping= -42.5332848 eV
 O Al  O Al  O Al  O Os
 1.0000000000000000
     8.1252428492400028    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1252428492400028    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.0213966198119593
  18  12  24  16  12   8   2  45
Selective dynamics
Cartesian
  3.2991912187556491  7.2937851792404542 10.9423958550990683   F   F   F
  7.4580655726235303  4.9860759177604841  9.3854545373318210   F   F   F
  3.3001893815290155  6.9406864361766143  8.0000187449185951   F   F   F
  3.3958161689947715  3.1340947240615882  8.1990827428381010   F   F   F
  7.3627977056619249  1.1795248166082488  9.5845317789161726   F   F   F
  3.3890000976188133  2.9482450895698054 10.8220669229527680   F   F   F
  0.6618814033949375  3.1341734237544863  8.1993257849376384   F   F   F
  4.8200971285871885  1.1794232564928941  9.5846030099037201   F   F   F
  0.6690703814507163  2.9481214281409560 10.8217845066302907   F   F   F
  0.7585343175343413  7.2938904994894243 10.9423584978630899   F   F   F
  4.7240141799275719  4.9861628008527772  9.3853700880230981   F   F   F
  0.7574411950172799  6.9404356788656125  7.9999999999999991   F   F   F
  6.0911850042196027  7.1185373383441490 10.9172067463060003   F   F   F
  6.0911425489618907  7.2238124231900196  8.0327436308783255   F   F   F
  2.0291658578723446  0.8962734802347320  9.5519775531218265   F   F   F
  2.0290554075975726  5.1995854453469219  9.4220834377914784   F   F   F
  6.0912751875555449  2.9204934754765293  8.1626394660302282   F   F   F
  6.0913560693206579  3.0216959978649696 10.8301543211852653   F   F   F
  0.6100845714845674  4.9805808209196227  8.0560139425344559   F   F   F
  4.6727336646281241  3.1397264995777956  9.5285274732362595   F   F   F
  0.6380002004711838  1.1125998084477480 10.9191009939757393   F   F   F
  7.5099560474594824  3.1396737190611170  9.5284873332419124   F   F   F
  3.4196019411544536  1.1126596869431156 10.9192047381793635   F   F   F
  3.4473258585825284  4.9805048495363664  8.0559839586400095   F   F   F
  6.0910306492314872  1.0189594823632340  8.1168144920444938   F   F   F
  6.0913909175176899  1.0181489132139694 10.8835529458276739   F   F   F
  6.0910970017651866  6.0565293682641990  9.4463612987341463   F   F   F
  2.0292348954960566  7.1011596512519830  9.4677862360962415   F   F   F
  2.0288978471091914  2.0636861277603167  8.1383270166926529   F   F   F
  2.0290068182983783  4.0513938745535549 10.8469192662674665   F   F   F
  3.2945294839706052  7.2156017154525403 16.5103250605651404   T   T   T
  7.4604315929227090  4.9767368491822568 14.9669090688816819   T   T   T
  3.3001893815290155  6.9406864361766143 13.5580397357678457   F   F   F
  7.4510903343308135  5.1717903799539169 12.3205669558782276   F   F   F
  7.3615344270772027  0.8264552864965863 12.2001224306209899   F   F   F
  3.3958161689947715  3.1340947240615882 13.7571037336873516   F   F   F
  7.3591234087889115  1.1707221272762249 15.1079725569553869   T   T   T
  3.3832441296699751  2.9268986993661774 16.3989070234773706   T   T   T
  4.8208359953704321  0.8263772733123053 12.2001609218852352   F   F   F
  0.6618814033949375  3.1341734237544863 13.7573467757868890   F   F   F
  4.8038950698116087  1.1759853321523628 15.0831620908816681   T   T   T
  0.6688493436370856  2.9220104916820908 16.3907599132899406   T   T   T
  0.7496094691686899  7.2126603301668180 16.4773502883386307   T   T   T
  4.7099975750987948  4.9696477885965891 14.9705723197050595   T   T   T
  0.7574411950172799  6.9404356788656125 13.5580209908492506   F   F   F
  4.7312500258749042  5.1717047227690971 12.3204488991888077   F   F   F
  6.0920368865077368  7.0708777925185782 16.5163663327207537   T   T   T
  6.0911425489618907  7.2238124231900196 13.5907646217275762   F   F   F
  2.0288417424237708  1.0016097555668855 12.2256103096605884   F   F   F
  2.0327708867020862  0.8612302283394410 15.0693407390744962   T   T   T
  2.0269357205881149  5.1758519112661707 14.9754721673915494   T   T   T
  2.0289241221255545  5.0983524375232827 12.3122395822918378   F   F   F
  6.0912751875555449  2.9204934754765293 13.7206604568794788   F   F   F
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6.0832003180723113	3.0035991429835600	16.4190073875141813	T	T	T
0.6100845714845674	4.9805808209196227	13.6140349333837065	F	F	F
4.7004630218670584	7.0073804319053679	12.2234202596149437	F	F	F
4.6685700184438570	3.1355651520683945	15.0918936081679629	T	T	T
0.6507660088260728	1.0647412349441194	16.3630080759378771	T	T	T
7.4994182366341562	3.1456755081684848	15.0948662349671121	T	T	T
3.4238985546456306	1.0643418041793515	16.4312882891359990	T	T	T
3.4473258585825284	4.9805048495363664	13.6140049494892601	F	F	F
7.4820144517446545	7.0074388210053060	12.2233730105456431	F	F	F
6.0910306492314872	1.0189594823632340	13.6748354828937444	F	F	F
6.0544641334631235	1.0251045452052958	16.4424847994895913	T	T	T
6.0787835470973324	6.0621051150017724	15.0212280882076463	T	T	T
2.0455721425698949	7.0523440566921076	15.0556749280086795	T	T	T
2.0287734206740944	7.1022039208828218	12.2590327337071869	F	F	F
2.0288978471091914	2.0636861277603167	13.6963480075419035	F	F	F
2.0275842711996654	4.0510999555472802	16.4081760766933513	T	T	T
6.0911678864681269	4.0685815256876436	12.2955930440659955	F	F	F
3.3656927600198281	6.8874446858777896	19.1487681013475424	T	T	T
7.3860551461466164	5.0965397977331861	17.9921043198252271	T	T	T
7.4426948767319585	0.8148554838264541	17.6188129843581081	T	T	T
3.2932049577825029	3.1877416469037021	19.3846205823928202	T	T	T
4.7482571476631081	0.8160580879890500	17.6454673269635585	T	T	T
0.6851851625060075	3.1935995313651535	19.3760001994316333	T	T	T
0.6603148288863766	6.8641668203416595	19.0792089940390888	T	T	T
4.8293769162711939	5.1813488173302824	18.0777191479131289	T	T	T
6.1514386543939921	7.4898528441096852	19.2332336388797209	T	T	T
1.9982717215532377	0.9425040157011324	17.6781336530279773	T	T	T
2.0329413964245564	5.0790443155962715	17.9049408568466433	T	T	T
6.1057481378817835	2.7021655816188641	19.3075968439157037	T	T	T
0.5888640220848615	4.9676051494309199	19.1608993883873566	T	T	T
4.7443946736182561	7.0975339885867879	17.9059587299153016	T	T	T
3.4560624203765276	4.9631820122429380	19.1582129932682257	T	T	T
7.4782630028596921	6.9164447370976649	17.7378837259387225	T	T	T
6.8678457477151396	1.0850205248989022	19.2805312022519075	T	T	T
2.0346853071286661	7.1157394579488145	17.8879014156598437	T	T	T
1.9739423246380332	1.9538438610963491	19.1258777489820417	T	T	T
6.0618989087648005	3.9267166633262662	17.9757391768169228	T	T	T
3.1679282054948579	1.0052592342896696	20.1321212583025719	T	T	T
8.6017859945429134	1.0097734349694818	20.0037276803659800	T	T	T
0.5614028698941587	-0.5071042133153340	21.3789105783221878	T	T	T
1.9300150329518342	1.0160081567208050	23.1473362187495653	T	T	T
0.5663855810419970	-0.3000290597095438	25.2365135901393494	T	T	T
0.5379821034725177	2.5577598154132857	21.4178109011042146	T	T	T
1.9357090003360802	3.6698971821857640	23.3590284317204926	T	T	T
0.5667237793787513	2.3639669805976671	25.2394473045735204	T	T	T
0.5652496552955543	5.1014396039958854	21.6838875843012993	T	T	T
1.9361033816000333	6.5071539272949490	23.3649476649070955	T	T	T
0.5750378156581452	5.0941879479581722	25.2666319101397043	T	T	T
3.2948087371037156	-0.4993660256332801	21.3542059386660306	T	T	T
4.6372892744273848	1.0101963050175111	23.1404071414111812	T	T	T
3.2826014915721675	-0.2973618409989540	25.2369925196206282	T	T	T
3.3260608827041431	2.5468404104802613	21.4091518724498293	T	T	T
4.6517330009035831	3.7059916952475893	23.3643084400585188	T	T	T
3.2793911800946289	2.3606428941619120	25.2429314578823849	T	T	T
3.2797826545757847	5.0999751329053398	21.6735672587133408	T	T	T
4.6490111382476300	6.4704923073539327	23.3520456254796791	T	T	T
3.2861625444118583	5.0939340058009765	25.2646311341243006	T	T	T
5.9937470223195239	-0.4322635104927569	21.3951323748209497	T	T	T
7.3464268333517282	1.0162876389486870	23.1538305876513881	T	T	T
5.9840406699933393	-0.3020914648970294	25.2509074942593514	T	T	T
5.9841737773627832	2.4864632517449485	21.4126654973993276	T	T	T
7.3197131107520059	3.6849584911359328	23.3524432725335949	T	T	T
5.9850753665951633	2.3508345040359351	25.2519453106031087	T	T	T

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  5.9932808054828204  5.0914907894836885 21.5554432974434391   T   T   T
  7.3246657303773750  6.4980158300324771 23.3426723437165293   T   T   T
  5.9920037896206528  5.0944511687170140 25.2838091796237059   T   T   T
  1.9290581176526505  1.0271892690507551 27.1965714340332383   T   T   T
  0.5727287285423605 -0.3324422483081591 29.0160048419052110   T   T   T
  1.9234166845852616  3.7209993482219352 27.1779853513170124   T   T   T
  0.5723505837308428  2.3848508503309631 29.0158477606831795   T   T   T
  1.9237675557179623  6.4535703479820636 27.1801400847707342   T   T   T
  0.5773555461942155  5.0891100750391454 28.9912847103821143   T   T   T
  4.6333155672156838  1.0316593637411835 27.2305845820243206   T   T   T
  3.2733049801490361 -0.3343422443795231 29.0167861258588289   T   T   T
  4.6300693634995485  3.7272043491286784 27.1889436769040316   T   T   T
  3.2721287745340968  2.3891913981731583 29.0185306406778487   T   T   T
  4.6299947828897503  6.4560522067326165 27.1901959388619439   T   T   T
  3.2744370375586516  5.0905657823879142 28.9926090859291818   T   T   T
  7.3374348174187993  1.0282592762675056 27.2215878260512945   T   T   T
  5.9914227096757529 -0.3313930814532961 29.0191099749585710   T   T   T
  7.3474978346354227  3.7243313457823111 27.1779582013122187   T   T   T
  5.9930312974027906  2.3895191712897592 29.0208702181042817   T   T   T
  7.3482456295473524  6.4538068966310016 27.1814332483611203   T   T   T
  5.9871629614736852  5.0931566486284936 28.9806249253758565   T   T   T

Oxide reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Os E_tot= -694.26886514 eV
 D3-zero damping= -11.1393653 eV, D3-BJ damping= -16.7404879 eV
 O Al  O Al  O Al  H  O  H  O  H
 1.0000000000000000
     8.1252428492400028    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1252428492400028    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6840463963622163
  18  12  24  16  12   8   1   1   1   1   2
Selective dynamics
Cartesian
  3.2991912187556491  7.2937851792404542 10.9423958550990683   F   F   F
  7.4580655726235303  4.9860759177604841  9.3854545373318210   F   F   F
  3.3001893815290155  6.9406864361766143  8.0000187449185951   F   F   F
  3.3958161689947715  3.1340947240615882  8.1990827428381010   F   F   F
  7.3627977056619249  1.1795248166082488  9.5845317789161726   F   F   F
  3.3890000976188133  2.9482450895698054 10.8220669229527680   F   F   F
  0.6618814033949375  3.1341734237544863  8.1993257849376384   F   F   F
  4.8200971285871885  1.1794232564928941  9.5846030099037201   F   F   F
  0.6690703814507163  2.9481214281409560 10.8217845066302907   F   F   F
  0.7585343175343413  7.2938904994894243 10.9423584978630899   F   F   F
  4.7240141799275719  4.9861628008527772  9.3853700880230981   F   F   F
  0.7574411950172799  6.9404356788656125  8.0000000000000000   F   F   F
  6.0911850042196027  7.1185373383441490 10.9172067463060003   F   F   F
  6.0911425489618907  7.2238124231900196  8.0327436308783255   F   F   F
  2.0291658578723446  0.8962734802347320  9.5519775531218265   F   F   F
  2.0290554075975726  5.1995854453469219  9.4220834377914784   F   F   F
  6.0912751875555449  2.9204934754765293  8.1626394660302282   F   F   F
  6.0913560693206579  3.0216959978649696 10.8301543211852653   F   F   F
  0.6100845714845674  4.9805808209196227  8.0560139425344559   F   F   F
  4.6727336646281241  3.1397264995777956  9.5285274732362595   F   F   F
  0.6380002004711838  1.1125998084477480 10.9191009939757393   F   F   F
  7.5099560474594824  3.1396737190611170  9.5284873332419124   F   F   F
  3.4196019411544536  1.1126596869431156 10.9192047381793635   F   F   F
  3.4473258585825284  4.9805048495363664  8.0559839586400095   F   F   F
  6.0910306492314872  1.0189594823632340  8.1168144920444938   F   F   F
  6.0913909175176899  1.0181489132139694 10.8835529458276739   F   F   F
  6.0910970017651866  6.0565293682641990  9.4463612987341463   F   F   F
  2.0292348954960566  7.1011596512519830  9.4677862360962415   F   F   F
  2.0288978471091914  2.0636861277603167  8.1383270166926529   F   F   F
  2.0290068182983783  4.0513938745535549 10.8469192662674665   F   F   F
  3.2903646220643941  7.3149279298302883 16.5918080834345680   T   T   T
```

7.4652457497695135	4.9627455653117112	14.9618430597633090	T	T	T
3.3001893815290155	6.9406864361766143	13.5580397357678457	F	F	F
7.4510903343308135	5.1717903799539169	12.3205669558782276	F	F	F
7.3615344270772027	0.8264552864965863	12.2001224306209899	F	F	F
3.3958161689947715	3.1340947240615882	13.7571037336873516	F	F	F
7.3913699943689366	1.1512722434238476	15.1071662646134932	T	T	T
3.4038511652101682	2.9315110042764996	16.3910426179365913	T	T	T
4.8208359953704321	0.8263772733123053	12.2001609218852352	F	F	F
0.6618814033949375	3.1341734237544863	13.7573467757868890	F	F	F
4.7952444547863182	1.1550153249795794	15.1024255886789405	T	T	T
0.6380103319266608	2.9320441144467986	16.4078910820879358	T	T	T
0.7909533640873428	7.3108368640021313	16.5993492192589081	T	T	T
4.7157933501591289	4.9662527512738937	14.9629196152398940	T	T	T
0.7574411950172799	6.9404356788656125	13.5580209908492506	F	F	F
4.7312500258749042	5.1717047227690971	12.3204488991888077	F	F	F
6.0842017801374189	7.1139249117864054	16.4587538300519363	T	T	T
6.0911425489618907	7.2238124231900196	13.5907646217275762	F	F	F
2.0288417424237708	1.0016097555668855	12.2256103096605884	F	F	F
2.0254628759907214	0.9020553291622726	15.1399047904786013	T	T	T
2.0268516903889413	5.2038461689313174	14.9809927126414966	T	T	T
2.0289241221255545	5.0983524375232827	12.3122395822918378	F	F	F
6.0912751875555449	2.9204934754765293	13.7206604568794788	F	F	F
6.0928998256936042	2.9618695286454333	16.3357167942512476	T	T	T
0.6100845714845674	4.9805808209196227	13.6140349333837065	F	F	F
4.7004630218670584	7.0073804319053679	12.2234202596149437	F	F	F
4.6806810330152775	3.1225192914060371	15.0698187927165748	T	T	T
0.6424054041785866	1.1068642590248983	16.5187181488238402	T	T	T
7.5021972941811113	3.1169254861311617	15.0654713687357926	T	T	T
3.4029462695610424	1.1124381630817990	16.4909203823749415	T	T	T
3.4473258585825284	4.9805048495363664	13.6140049494892601	F	F	F
7.4820144517446545	7.0074388210053060	12.2233730105456431	F	F	F
6.0910306492314872	1.0189594823632340	13.6748354828937444	F	F	F
6.0941140340384781	0.9474307999313684	16.3871537670879022	T	T	T
6.0920522270948547	6.0591713475665587	15.0020490482658069	T	T	T
2.0257356345893278	7.0938966879450325	15.1018603352606142	T	T	T
2.0287734206740944	7.1022039208828218	12.2590327337071869	F	F	F
2.0288978471091914	2.0636861277603167	13.6963480075419035	F	F	F
2.0235755552358858	4.0075531675843061	16.3269648171089443	T	T	T
6.0911678864681269	4.0685815256876436	12.2955930440659955	F	F	F
3.4094450150444913	6.6872574053834253	19.1262991615435602	T	T	T
7.4033696290980222	5.1342488220490665	17.8640742517626094	T	T	T
7.3827815413060618	0.8416459241926345	17.7346361008387632	T	T	T
3.3744314293065889	3.3471191461253857	19.7380105941854254	T	T	T
4.7767273996309880	0.9047652169591437	17.7030607735541956	T	T	T
0.6279462407649462	3.3601089196892575	19.6788993318956145	T	T	T
0.7006966581789539	6.7405442818533032	19.1630038648422385	T	T	T
4.8395734593996682	5.0591027880603878	17.8705455562808488	T	T	T
6.0855964394678859	7.3290450258520465	19.0776320517555220	T	T	T
2.0199320991746830	1.0956403600337372	17.9352842947944353	T	T	T
2.0515526224740799	4.9196628877528532	17.8416488879384687	T	T	T
6.3863555087101931	2.7964970915602456	19.1865501709675748	T	T	T
0.6275211322327501	4.9404137526902829	18.9281912799541203	T	T	T
4.7512851133047898	6.9354661459987597	17.8421528414691544	T	T	T
3.4915345478329489	4.8736034223022324	18.9357583978115755	T	T	T
7.4546539888909296	7.0109656950746615	17.8751278293349429	T	T	T
5.9416822502644990	1.0056586668184793	19.0909658764705199	T	T	T
2.0540103590985570	7.2814187989899724	18.0674432473888551	T	T	T
2.0059371119760372	2.2244246918780251	19.5166891036804202	T	T	T
6.1523215711730233	3.9287381838225492	17.8075283588510338	T	T	T
7.4005407988056930	2.9606016485269482	19.5013796309850456	T	T	T
2.1901047534792366	0.9837745985203059	20.7386663436373233	T	T	T
1.7099058101367599	0.1404676740979864	20.6701401793991586	T	T	T
4.8348462013696336	1.3025314268563046	20.5741309663564564	T	T	T

```
  4.4642683005031758  2.2437953000771906 20.4413527656027405   T   T   T
  3.9839187250919830  0.7837349527391814 20.7266073459702262   T   T   T

Metal reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Os E_tot= -488.15993705 eV
 D3-zero damping= -19.0922672 eV, D3-BJ damping= -21.8257468 eV
Os
 1.0000000000000000
     8.1252428492400028    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1252428492400028    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0003327350601025 -0.0003346110310579  8.0726608277313492
  1.3538741175768974  1.3538740377712515  9.8838688012508111
 -0.0006213215287964 -0.0006210867386008 11.8277583989553854
  1.3535311440795212  1.3535335993101891 13.7715187921730688
 -0.0005808773649082 -0.0005834559026537 15.5827451483542401
 -0.0003323445937836  2.7076544285264514  8.0732543411712410
  1.3543135741350174  4.0623965012208352  9.8837887839751914
 -0.0005423914076921  2.7069404646696054 11.8277878366031324
  1.3541164706629185  4.0621066987414727 13.7715053263847196
 -0.0006586889950677  2.7073242333342296 15.5822488874604392
 -0.0002858251922651  5.4170370500658542  8.0731254457831980
  1.3539231961714231  6.7706584245364247  9.8838735619162410
 -0.0005854772143716  5.4170201526163160 11.8277866499189699
  1.3535388553480701  6.7702221242674741 13.7715310128444095
 -0.0006372923742848  5.4166299816664107 15.5823986643507642
  2.7076516850455947 -0.0003376291575535  8.0732515812766596
  4.0623958434547927  1.3543131476028316  9.8837901606286280
  2.7069405945475418 -0.0005428192943669 11.8277862506751053
  4.0621072620845462  1.3541172696110015 13.7715052064373129
  2.7073242787840943 -0.0006511975470205 15.5822455137109426
  2.7078991734544395  2.7078980565888213  8.0727266992488467
  4.0622935495383343  4.0622923645163285  9.8839738267261730
  2.7078347901388775  2.7078340720111571 11.8274777234662594
  4.0619818682628734  4.0619814396579681 13.7711806560253187
  2.7076553141432975  2.7076530587817005 15.5827338662937347
  2.7079594460400527  5.4166936362165821  8.0727080847598991
  4.0624567149622823  6.7703925099470226  9.8837740266492986
  2.7079024773733575  5.4165755562285760 11.8276483467345610
  4.0620622375568081  6.7701782285959959 13.7717319605329021
  2.7077365319745326  5.4162004974683100 15.5827929677851991
  5.4170413067926946 -0.0002732559020941  8.0731269910536980
  6.7706604413520886  1.3539216229925839  9.8838737606823859
  5.4170202257646487 -0.0005850191989876 11.8277870458024292
  6.7702225494835302  1.3535374565553151 13.7715324055711577
  5.4166239759709134 -0.0006470149525163 15.5824011821692974
  5.4166921840754938  2.7079567599721308  8.0727073119501362
  6.7703916888686306  4.0624572106795451  9.8837762768263548
  5.4165744015979689  2.7079035335379755 11.8276495651922033
  6.7701777117316402  4.0620635705562993 13.7717321305535734
  5.4162010443114701  2.7077400368276767 15.5827914657268316
  5.4166622873822519  5.4166588459954994  8.0726629005991715
  6.7706673226347904  6.7706674785178897  9.8838693572360121
  5.4163504590435467  5.4163489836779357 11.8277907793031254
  6.7702378199766589  6.7702388689936583 13.7716573034948766
  5.4162006871495878  5.4162004123205847 15.5828540873254884

Interface: 2O-g-Al2O3(110)/fcc(100)_3x3/Ru E_tot= -1089.55964653 eV
 D3-zero damping= -33.8260131 eV, D3-BJ damping= -42.4072886 eV
 O Al  O Al  O Al  O Ru
 1.0000000000000000
     7.9985842258200019    0.0000000000000000    0.0000000000000000
```

```
     0.0000000000000000    7.9985842258200019    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.2716937760818396
  18  12  24  16  12   8   2  45
Selective dynamics
Cartesian
  3.2477624767573676  7.1800875572167371 10.9423958550990683   F   F   F
  7.3418071005591603  4.9083515317047208  9.3854545373318210   F   F   F
  3.2487450798822204  6.8324930189573090  8.0000187449185951   F   F   F
  3.3428812094701477  3.0852395537260136  8.1990827428381010   F   F   F
  7.2480242965192909  1.1611380443808434  9.5845317789161726   F   F   F
  3.3361713889759947  2.9022869968114313 10.8220669229527680   F   F   F
  0.6515638056348727  3.0853170266254546  8.1993257849376384   F   F   F
  4.7449600676543389  1.1610380674137890  9.5846030099037201   F   F   F
  0.6586407198322246  2.9021652630525163 10.8217845066302907   F   F   F
  0.7467100663386105  7.1801912357033624 10.9423584978630899   F   F   F
  4.6503748876444915  4.9084370604383718  9.3853700880230981   F   F   F
  0.7456339837298706  6.8322461705234216  8.0000000000000000   F   F   F
  5.9962338597497276  7.0075715300885992 10.9172067463060003   F   F   F
  5.9961920662967882  7.1112055566209627  8.0327436308783255   F   F   F
  1.9975346366254598  0.8823021113389700  9.5519775531218265   F   F   F
  1.9974259080813512  5.1185328113417841  9.4220834377914784   F   F   F
  5.9963226372818808  2.8749679828636467  8.1626394660302282   F   F   F
  5.9964022582387670  2.9745929312139707 10.8301543211852653   F   F   F
  0.6005743976438872  4.9029420940145254  8.0560139425344559   F   F   F
  4.5998937477725370  3.0907835395050367  9.5285274732362595   F   F   F
  0.6280548697736621  1.0952562825039629 10.9191009939757393   F   F   F
  7.3928886917428587  3.0907315817462386  9.5284873332419124   F   F   F
  3.3662962021694955  1.0953152275961158 10.9192047381793635   F   F   F
  3.3935879511956646  4.9028673068950512  8.0559839586400095   F   F   F
  5.9960819108915793  1.0030756487656995  8.1168144920444938   F   F   F
  5.9964365632120771  1.0022777150015598 10.8835529458276739   F   F   F
  5.9961472291028919  5.9621184458191046  9.4463612987341463   F   F   F
  1.9976025980708296  6.9904647313829278  9.4677862360962415   F   F   F
  1.9972708036911981  2.0315167946138590  8.1383270166926529   F   F   F
  1.9973780762061333  3.9882395811245073 10.8469192662674665   F   F   F
  3.2549050323918447  7.1238657584732357 16.5712078202211899   T   T   T
  7.3609800736047797  4.9117717207412293 14.9817054554868694   T   T   T
  3.2487450798822204  6.8324930189573090 13.5580397357678457   F   F   F
  7.3349405942879429  5.0911710234256331 12.3205669558782276   F   F   F
  7.2467807102846322  0.8135722636936886 12.2001224306209899   F   F   F
  3.3428812094701477  3.0852395537260136 13.7571037336873516   F   F   F
  7.2739254679618606  1.1298238880502898 15.1070665317830493   T   T   T
  3.3396874733629787  2.8953937753314718 16.4326788668645563   T   T   T
  4.7456874167695702  0.8134954666013710 12.2001609218852352   F   F   F
  0.6515638056348727  3.0853170266254546 13.7573467757868890   F   F   F
  4.7143075212258916  1.1290214438078914 15.1160722588938636   T   T   T
  0.6606811040441997  2.8899903313504947 16.4228393165178161   T   T   T
  0.7366723679431743  7.1109726419676704 16.5530501934821359   T   T   T
  4.6321942743564515  4.9099039321951707 14.9811654752964323   T   T   T
  0.7456339837298706  6.8322461705234216 13.5580209908492506   F   F   F
  4.6574979391432185  5.0910867014896573 12.3204488991888077   F   F   F
  5.9906141930955537  6.9856574448936986 16.5161050917930616   T   T   T
  5.9961920662967882  7.1112055566209627 13.5907646217275762   F   F   F
  1.9972155735817569  0.9859963745027107 12.2256103096605884   F   F   F
  2.0027739735275332  0.8567221683704913 15.1045249890137914   T   T   T
  1.9998686003083450  5.1032681200827597 15.0063624402035174   T   T   T
  1.9972966691250460  5.0188778527719968 12.3122395822918378   F   F   F
  5.9963226372818808  2.8749679828636467 13.7206604568794788   F   F   F
  5.9953136572826784  2.9501358786547001 16.4074008819772814   T   T   T
  0.6005743976438872  4.9029420940145254 13.6140349333837065   F   F   F
  4.6271908518122293  6.8981473694906974 12.2234202596149437   F   F   F
  4.5969334694342416  3.0954143304607489 15.1067478103143511   T   T   T
  0.6363422690652638  1.0512445539342472 16.4314219191177777   T   T   T
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7.3942943692178984	3.0981502660613547	15.1085702770348345	T	T	T
3.3689128869310059	1.0599499512043409	16.4648013693954738	T	T	T
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1.9971483168511726	6.9914927226382924	12.2590327337071869	F	F	F
1.9972708036911981	2.0315167946138590	13.6963480075419035	F	F	F
1.9973492094304330	4.0303624284542270	16.4636242254951988	T	T	T
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7.2811641831401861	5.0165542357551107	18.0267828071773479	T	T	T
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4.7224157748728048	0.8584885319734217	17.7388622404454495	T	T	T
0.6044241496576624	3.0525449890121537	19.4914484547139786	T	T	T
0.6287768991244024	6.8014757775359271	19.1819238020414176	T	T	T
4.6625118686594522	5.0437175873824023	18.0265731390775201	T	T	T
5.9655403666014264	7.2217236790895898	19.1581346961170418	T	T	T
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5.8959316452948896	2.7967130984834734	19.3486320672344299	T	T	T
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7.3297180921867611	6.8440523616316522	17.8725744418197081	T	T	T
6.1021204257007389	1.0657638953111570	19.0502096311427209	T	T	T
1.9842148852517798	7.0128993421769943	17.9970359374571949	T	T	T
1.9721427851554090	2.0456787591000198	19.1115623240264618	T	T	T
5.9566522723879718	3.8775345142775417	17.9635419535819345	T	T	T
2.0390838342346633	0.9143659125619603	20.4769944966971416	T	T	T
7.1877193788282820	0.9822521403695947	20.5510160984568806	T	T	T
0.6071725187182050	-0.3354562780593316	21.4476553853231771	T	T	T
1.9290186996929837	1.0682003836007368	23.3571004670082694	T	T	T
0.5881917951797216	-0.2605422307273318	25.2864922283462157	T	T	T
0.5607750201222377	2.5200933712056113	21.5584756446366441	T	T	T
1.9136642485174498	3.6832372479493585	23.4186510393968739	T	T	T
0.5886092033546240	2.3915543442553444	25.2819828657173566	T	T	T
0.6033046348312260	5.0927030215556801	21.7658527007993250	T	T	T
1.9308709191632314	6.4779023603956025	23.4355590653346262	T	T	T
0.5942944974728769	5.0785736537575490	25.3092358390700625	T	T	T
3.3234102719268952	-0.3882717082461755	21.4318061894269114	T	T	T
4.5939341481091844	1.0444152581985859	23.2930726126922814	T	T	T
3.2633082910270743	-0.2457320663355503	25.2946776224287149	T	T	T
3.2865711444117798	2.4880260391252591	21.5580088298445283	T	T	T
4.6061282892667332	3.6994463387301373	23.3984588255536003	T	T	T
3.2638857926750036	2.4011606907878380	25.2985469796457139	T	T	T
3.2517384208362761	5.0759880720161421	21.7663195945558741	T	T	T
4.6149981539484646	6.4104140916536210	23.4262381069569017	T	T	T
3.2634804256205876	5.0842631571353518	25.3511400049118478	T	T	T
5.8940707047268983	-0.3799907282396214	21.4728371190051526	T	T	T
7.2428573191816144	1.0662007406275158	23.3805180527759866	T	T	T
5.9200458730661962	-0.2482925136593559	25.3015107598426248	T	T	T
5.9007239075813196	2.4885000292524122	21.4983229935685003	T	T	T
7.2366039938000881	3.7181269605297889	23.3940576450592665	T	T	T
5.9247863841457029	2.3951849468252084	25.3021087772289270	T	T	T
5.9189644055234041	5.0742301604737037	21.6338712904905854	T	T	T
7.2433421452956770	6.4264875902663183	23.4198810540497533	T	T	T
5.9240350142346516	5.0787026419617929	25.3446788901494884	T	T	T
1.9271159620619649	1.0784877812832698	27.2099766837371462	T	T	T
0.5933595737046030	-0.2611805911803890	29.0195045339145352	T	T	T

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  1.9294415115379444  3.7380445029603746 27.1988955111067057   T   T   T
  0.5964362814027367  2.4092898701844661 29.0210106632161242   T   T   T
  1.9280244963341413  6.4015315590290598 27.2087446204360646   T   T   T
  0.5900797631509260  5.0696225838319879 29.0079611237903521   T   T   T
  4.5934507951474526  1.0784537041430504 27.2215179112914818   T   T   T
  3.2566428409738868 -0.2439646117455905 29.0193299340445492   T   T   T
  4.5851899639414091  3.7543413683792028 27.2210080611054863   T   T   T
  3.2541640608143050  2.3985625385033038 29.0197582268934866   T   T   T
  4.5841616660701394  6.4035977420295866 27.2367710070904820   T   T   T
  3.2445183259034169  5.0641656363554777 29.0125533364804191   T   T   T
  7.2604640383647236  1.0764725647331939 27.2318981054843583   T   T   T
  5.9289932600428887 -0.2464756475486501 29.0241672015549454   T   T   T
  7.2548789922600054  3.7363928667793709 27.1974815097721709   T   T   T
  5.9314408703557655  2.4070294558960303 29.0225559588206821   T   T   T
  7.2549418014166900  6.4075503784071106 27.2098589280914140   T   T   T
  5.9390731118421103  5.0671448388896758 29.0089693945990987   T   T   T

Oxide reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Ru E_tot= -693.01715806 eV
 D3-zero damping= -11.4603209 eV, D3-BJ damping= -17.2108296 eV
 O Al  O Al  O Al  H  O  H  O  H
 1.0000000000000000
     7.9985842258200019    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.9985842258200019    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6840463963622163
  18  12  24  16  12   8   1   1   1   1   2
Selective dynamics
Cartesian
  3.2477624767573676  7.1800875572167371 10.9423958550990683   F   F   F
  7.3418071005591603  4.9083515317047208  9.3854545373318210   F   F   F
  3.2487450798822204  6.8324930189573090  8.0000187449185951   F   F   F
  3.3428812094701477  3.0852395537260136  8.1990827428381010   F   F   F
  7.2480242965192909  1.1611380443808434  9.5845317789161726   F   F   F
  3.3361713889759947  2.9022869968114313 10.8220669229527680   F   F   F
  0.6515638056348727  3.0853170266254546  8.1993257849376384   F   F   F
  4.7449600676543389  1.1610380674137890  9.5846030099037201   F   F   F
  0.6586407198322246  2.9021652630525163 10.8217845066302907   F   F   F
  0.7467100663386105  7.1801912357033624 10.9423584978630899   F   F   F
  4.6503748876444915  4.9084370604383718  9.3853700880230981   F   F   F
  0.7456339837298706  6.8322461705234216  8.0000000000000000   F   F   F
  5.9962338597497276  7.0075715300885992 10.9172067463060003   F   F   F
  5.9961920662967882  7.1112055566209627  8.0327436308783255   F   F   F
  1.9975346366254598  0.8823021113389700  9.5519775531218265   F   F   F
  1.9974259080813512  5.1185328113417841  9.4220834377914784   F   F   F
  5.9963226372818808  2.8749679828636467  8.1626394660302282   F   F   F
  5.9964022582387670  2.9745929312139707 10.8301543211852653   F   F   F
  0.6005743976438872  4.9029420940145254  8.0560139425344559   F   F   F
  4.5998937477725370  3.0907835395050367  9.5285274732362595   F   F   F
  0.6280548697736621  1.0952562825039629 10.9191009939757393   F   F   F
  7.3928886917428587  3.0907315817462386  9.5284873332419124   F   F   F
  3.3662962021694955  1.0953152275961158 10.9192047381793635   F   F   F
  3.3935879511956646  4.9028673068950512  8.0559839586400095   F   F   F
  5.9960819108915793  1.0030756487656995  8.1168144920444938   F   F   F
  5.9964365632120771  1.0022777150015598 10.8835529458276739   F   F   F
  5.9961472291028919  5.9621184458191046  9.4463612987341463   F   F   F
  1.9976025980708296  6.9904647313829278  9.4677862360962415   F   F   F
  1.9972708036911981  2.0315167946138590  8.1383270166926529   F   F   F
  1.9973780762061333  3.9882395811245073 10.8469192662674665   F   F   F
  3.2452964755303313  7.1800536949193683 16.6264970348472758   T   T   T
  7.3589790558121981  4.8981402071869420 14.9765491477458106   T   T   T
  3.2487450798822204  6.8324930189573090 13.5580397357678457   F   F   F
  7.3349405942879429  5.0911710234256331 12.3205669558782276   F   F   F
  7.2467807102846322  0.8135722636936886 12.2001224306209899   F   F   F
  3.3428812094701477  3.0852395537260136 13.7571037336873516   F   F   F
```

7.2885605707373582	1.1176199188241382	15.1235241819992385	T	T	T
3.3548374339726972	2.9012231794311854	16.4180321157939773	T	T	T
4.7456874167695702	0.8134954666013710	12.2001609218852352	F	F	F
0.6515638056348727	3.0853170266254546	13.7573467757868890	F	F	F
4.7097490480443955	1.1213531503743546	15.1199487315158905	T	T	T
0.6240537674849486	2.9025276550746644	16.4368085119797307	T	T	T
0.7765207378883904	7.1785530991473374	16.6357245797881426	T	T	T
4.6340421284742250	4.9022364069539988	14.9766670215760840	T	T	T
0.7456339837298706	6.8322461705234216	13.5580209908492506	F	F	F
4.6574979391432185	5.0910867014896573	12.3204488991888077	F	F	F
5.9936961720148805	7.0031056030787635	16.4912463455155240	T	T	T
5.9961920662967882	7.1112055566209627	13.5907646217275762	F	F	F
1.9972155735817569	0.9859963745027107	12.2256103096605884	F	F	F
1.9946446079394491	0.8891732423294133	15.1622190006731934	T	T	T
1.9959294486882422	5.1230858186285717	14.9986529655800691	T	T	T
1.9972966691250460	5.0188778527719968	12.3122395822918378	F	F	F
5.9963226372818808	2.8749679828636467	13.7206604568794788	F	F	F
5.9991297932513872	2.9113167527061172	16.3500403006140900	T	T	T
0.6005743976438872	4.9029420940145254	13.6140349333837065	F	F	F
4.6271908518122293	6.8981473694906974	12.2234202596149437	F	F	F
4.6013257347960481	3.0745070124505558	15.0840245158110342	T	T	T
0.6372400184844967	1.0926627772309478	16.5526836008544755	T	T	T
7.3924326701461549	3.0678581321666147	15.0794341756328052	T	T	T
3.3479449191604513	1.0970044585614744	16.5249363630991830	T	T	T
3.3935879511956646	4.9028673068950512	13.6140049494892601	F	F	F
7.3653826576617032	6.8982048484045455	12.2233730105456431	F	F	F
5.9960819108915793	1.0030756487656995	13.6748354828937444	F	F	F
6.0000077419727855	0.9353996037257002	16.4126588368720299	T	T	T
5.9983962349003317	5.9869353582070000	15.0206444133028736	T	T	T
1.9949926309550916	6.9841556696990290	15.1146383531813946	T	T	T
1.9971483168511726	6.9914927226382924	12.2590327337071869	F	F	F
1.9972708036911981	2.0315167946138590	13.6963480075419035	F	F	F
1.9923532301678275	3.9843733571721378	16.3808843892118574	T	T	T
5.9962170088346873	4.0051593062072932	12.2955930440659955	F	F	F
3.3714799960698967	6.6024844353997860	19.1954742779086054	T	T	T
7.3080039158041288	5.0409124372580330	17.8942098001663865	T	T	T
7.2718527711259267	0.8445153022305550	17.7737341304947627	T	T	T
3.3254329545668382	3.2836345319651912	19.8404788526927121	T	T	T
4.6981003960523067	0.8975181909142508	17.7464224256987535	T	T	T
0.5995704298484523	3.2997308423566736	19.7765021727109165	T	T	T
0.6843609109656281	6.6600415420531753	19.2333440658656656	T	T	T
4.7495399347103024	4.9625125759945421	17.8980040479584979	T	T	T
5.9974270220172778	7.1897514126433375	19.1202169508879258	T	T	T
1.9915328400233883	1.0832951531924480	17.9808683504210052	T	T	T
2.0227123239605231	4.8521786531595863	17.9189363154242400	T	T	T
6.2642084518300649	2.7613738216649053	19.2476227352102178	T	T	T
0.6084497440641435	4.8690994753739734	19.0169821157990881	T	T	T
4.6779226665857703	6.8222557455754931	17.8737400367589920	T	T	T
3.4558936198511323	4.7956889921366592	19.0260932457208085	T	T	T
7.3449414526035399	6.9011345314781600	17.9065893115527608	T	T	T
5.8454718723418075	0.9821786935071586	19.1454543104195594	T	T	T
2.0266773240814415	7.1507873308421406	18.1079708087362299	T	T	T
1.9678014253255560	2.1578717131217244	19.5899455676939027	T	T	T
6.0609333510475203	3.8440592284351895	17.8352650404561537	T	T	T
7.2838451573020286	2.9247890945941348	19.5830509884810553	T	T	T
2.1158305322806199	0.9088681971883382	20.8023376033963423	T	T	T
1.6438276007504689	0.0644783523363264	20.6884480882020014	T	T	T
4.7687030506781873	1.2328374796867012	20.6580237603075290	T	T	T
4.3987609294277323	2.1763224881928469	20.5505837800724258	T	T	T
3.9210213677495838	0.7057851306179701	20.7971448953318543	T	T	T

Metal reference: 2O-g-Al2O3(110)/fcc(100)_3x3/Ru E_tot= -405.36638166 eV
D3-zero damping= -18.3989542 eV, D3-BJ damping= -21.5203814 eV

```
Ru
 1.0000000000000000
     7.9985842258200019    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.9985842258200019    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0038453081226937 -0.0004090309230234  8.1265508146813232
  1.3336832682896687  1.3332538190226704  9.9182356994329890
 -0.0000120299327283 -0.0003080689488928 11.8283961194142169
  1.3334964701589767  1.3332254513509585 13.7380356488609827
 -0.0018349130475245 -0.0043411702989405 15.5292313602483674
 -0.0007501370339095  2.6648461734405706  8.1209770823533773
  1.3327594926721886  3.9981485634376641  9.9174410603996694
 -0.0001741299985207  2.6665151789543224 11.8279891409823783
  1.3333301836930633  3.9988160419761281 13.7384648973183623
 -0.0001143182330345  2.6652580608646441 15.5343526279817148
 -0.0004826020321127  5.3336130020245731  8.1212219729904618
  1.3327846926936109  6.6638002002111998  9.9186428154775594
 -0.0000347841192725  5.3316258466738393 11.8275103737889271
  1.3341056398064759  6.6635775256955263 13.7357557688178780
 -0.0006038727371930  5.3330047555171065 15.5339359450231047
  2.6650699096514865 -0.0002253969042696  8.1202738013201863
  3.9984991651283228  1.3331158681288411  9.9166767775708085
  2.6668098524861081 -0.0000149974689690 11.8274764294360057
  3.9985892512010661  1.3331750770426378 13.7378705283150815
  2.6654303716887235 -0.0001553975964232 15.5344267610478646
  2.6636185907374448  2.6638848259855643  8.1201687730425434
  3.9991198765365974  3.9992760728780752  9.9185085779172972
  2.6660345851853267  2.6660897680477609 11.8277483464038493
  3.9990617586855839  3.9991701079187298 13.7361288066715659
  2.6633520957420957  2.6634720830853174 15.5352306371314377
  2.6634186163688018  5.3339441233049305  8.1200392423445376
  3.9980975690195106  6.6653542706119087  9.9176328052417873
  2.6663639032122366  5.3322103968300674 11.8272868278348113
  3.9989486692890752  6.6651058012433841 13.7387946478045073
  2.6640579638168123  5.3331283136935328 15.5351956676340457
  5.3336020350540041 -0.0000018789249453  8.1218611402136425
  6.6640486199010347  1.3342429738993893  9.9211930018591765
  5.3318321400964130 -0.0000166368529822 11.8280263699813144
  6.6640042984428112  1.3323335842284534 13.7373658420724158
  5.3329849746499178 -0.0005435519606291 15.5342149998015966
  5.3344214131441490  2.6641839059998689  8.1203505057087888
  6.6648616837131840  3.9989218086534581  9.9166519760450793
  5.3319792239929749  2.6664696242473140 11.8276671933943760
  6.6652072953531745  3.9977673965570308 13.7369358690993408
  5.3338521812397692  2.6639162017226563 15.5349001825971325
  5.3336856462435618  5.3349534450696501  8.1203853179516745
  6.6638636481564761  6.6643572865489480  9.9211916001911753
  5.3311417325205239  5.3315720763010024 11.8278292993229819
  6.6639313427553564  6.6636053739618371 13.7337967586346199
  5.3349340364375015  5.3332103024600821 15.5348227253362090

Interface: ZnO(10-10)/fcc(100)_6x2/Au E_tot= -480.03096122 eV
 D3-zero damping= -33.5953433 eV, D3-BJ damping= -32.1068342 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Au
 1.0000000000000000
    17.3925102628200072    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7975034209400009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.3241942887299736
```

```
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2  36
Selective dynamics
Cartesian
  3.4784166234049381  5.7920814396558580  8.9451241821253618   F   F   F
  1.7391677333950526  2.8933297495539323  8.0000001838787966   F   F   F
  3.4784171936104840  3.5940765006679847  8.9451248436730744   F   F   F
  1.7391667701727282  0.6953248071507115  8.0000000000000000   F   F   F
  1.7391704735109343  5.7920813601461925 11.7805090714841079   F   F   F
  3.4784236360650502  2.8933296700442663 10.8353850732375427   F   F   F
  1.7391710437164798  3.5940764211583196 11.7805097330318205   F   F   F
  3.4784226728427257  0.6953247276410457 10.8353848893587461   F   F   F
  3.4578465407451602  5.6669082419573673 14.3673233499701745   T   T   T
  1.7292526804899486  2.8376638968823369 13.6382545660409740   T   T   T
  3.4819496431045307  3.5949813051284893 14.3967884624365343   T   T   T
  1.7314632920549118  0.7013644192005984 13.6546597415098319   T   T   T
  1.7163892573370343  5.7110757021855445 16.9630299170901502   T   T   T
  3.4907873801365970  2.8192842756297090 16.3042414813730367   T   T   T
  1.7708147919750155  3.7174323125782540 16.8929458543206081   T   T   T
  3.4711577670654834  0.7403007183199654 16.2439771440424110   T   T   T
  6.9569186759689394  5.7920814396558580  8.9451241821253618   F   F   F
  5.2176697859590542  2.8933297495539323  8.0000001838787966   F   F   F
  6.9569192461744853  3.5940765006679847  8.9451248436730744   F   F   F
  5.2176688227367300  0.6953248071507115  8.0000000000000000   F   F   F
  5.2176725260749359  5.7920813601461925 11.7805090714841079   F   F   F
  6.9569256886290516  2.8933296700442663 10.8353850732375427   F   F   F
  5.2176730962804818  3.5940764211583196 11.7805097330318205   F   F   F
  6.9569247254067266  0.6953247276410457 10.8353848893587461   F   F   F
  6.9460486127811061  5.6563960017495125 14.3504496967639277   T   T   T
  5.2106059975443744  2.8189828707140276 13.6206044212219748   T   T   T
  6.9577923659544769  3.5866009887232746 14.3775228739739891   T   T   T
  5.2076747942167234  0.6920586097257826 13.6553737023617270   T   T   T
  5.1868040447102439  5.6961021676002597 16.8682430836207864   T   T   T
  6.9659024595874914  2.7937931335363291 16.2760384093193231   T   T   T
  5.2455529849645242  3.6919748353751429 16.8549838985385065   T   T   T
  6.9523326262773653  0.7234036327064871 16.2290982635215535   T   T   T
 10.4354207285329412  5.7920814396558580  8.9451241821253618   F   F   F
  8.6961718385230533  2.8933297495539323  8.0000001838787966   F   F   F
 10.4354212987384862  3.5940765006679847  8.9451248436730744   F   F   F
  8.6961708753007301  0.6953248071507115  8.0000000000000000   F   F   F
  8.6961745786389386  5.7920813601461925 11.7805090714841079   F   F   F
 10.4354277411930525  2.8933296700442663 10.8353850732375427   F   F   F
  8.6961751488444818  3.5940764211583196 11.7805097330318205   F   F   F
 10.4354267779707275  0.6953247276410457 10.8353848893587461   F   F   F
 10.4463933734428771  5.6560719866590805 14.3506355184833918   T   T   T
  8.6963224978324032  2.8159462419008481 13.6158845556140413   T   T   T
 10.4347865174031966  3.5865480536149961 14.3774578542201166   T   T   T
  8.6963602079353315  0.6882993421774969 13.6558365936936035   T   T   T
  8.6961369129716850  5.6917913961642643 16.8287942552526673   T   T   T
 10.4261972952851085  2.7937794831638421 16.2760562532171171   T   T   T
  8.6960319195050495  3.6814883208624272 16.8348457977936299   T   T   T
 10.4399797263083904  0.7234246044253991 16.2292084077882670   T   T   T
 13.9139227810969430  5.7920814396558580  8.9451241821253618   F   F   F
 12.1746738910870569  2.8933297495539323  8.0000001838787966   F   F   F
 13.9139233513024898  3.5940765006679847  8.9451248436730744   F   F   F
 12.1746729278647319  0.6953248071507115  8.0000000000000000   F   F   F
 12.1746766312029404  5.7920813601461925 11.7805090714841079   F   F   F
 13.9139297937570561  2.8933296700442663 10.8353850732375427   F   F   F
 12.1746772014084854  3.5940764211583196 11.7805097330318205   F   F   F
 13.9139288305347311  0.6953247276410457 10.8353848893587461   F   F   F
 13.9344737262233540  5.6668449015257787 14.3674820534401420   T   T   T
 12.1818828675684827  2.8189403342478410 13.6206159679692913   T   T   T
```

13.9104614796236454	3.5946829290447679	14.3969365375756642	T	T	T
12.1847619897687540	0.6919167624840280	13.6554197711136354	T	T	T
12.2053150636089320	5.6963460102646080	16.8691109657276535	T	T	T
13.9016247473629875	2.8194570854187719	16.3043638802525166	T	T	T
12.1465498207594251	3.6921352706881305	16.8551693595210104	T	T	T
13.9210352335369798	0.7403153426746012	16.2443563578276091	T	T	T
17.3924248336609466	5.7920814396558580	8.9451241821253618	F	F	F
15.6531759436510569	2.8933297495539323	8.0000001838787966	F	F	F
17.3924254038664898	3.5940765006679847	8.9451248436730744	F	F	F
15.6531749804287319	0.6953248071507115	8.0000000000000000	F	F	F
15.6531786837669387	5.7920813601461925	11.7805090714841079	F	F	F
17.3924318463210561	2.8933296700442663	10.8353850732375427	F	F	F
15.6531792539724854	3.5940764211583196	11.7805097330318205	F	F	F
17.3924308830987293	0.6953247276410457	10.8353848893587461	F	F	F
17.3926389327132291	5.6796278426703291	14.3890249298377135	T	T	T
15.6629332800337746	2.8372302386611103	13.6382208485408025	T	T	T
17.3923762961863702	3.6020016955224281	14.4316982212594205	T	T	T
15.6610492328778275	0.7011348604387972	13.6547321120390244	T	T	T
15.6755855193917064	5.7112830777432073	16.9633142370881416	T	T	T
17.3923924714950537	2.8574131867500041	16.3650753230648540	T	T	T
15.6216971262754445	3.7176361717966238	16.8931217111964180	T	T	T
17.3923206321837895	0.7562879914944152	16.2663400895562340	T	T	T
-0.0003261233180333	0.9303958528341819	19.1815702117984941	T	T	T
1.4401783889759505	2.3229983900033866	21.2815270288263712	T	T	T
-0.0004816465526498	0.8706637843403972	23.3759018574104580	T	T	T
-0.0020367506574054	3.8315290694731416	19.2442924333810090	T	T	T
1.4501211630581281	5.2317352181917842	21.2849764773624166	T	T	T
-0.0008070378418208	3.7716046465209221	23.3708640724585734	T	T	T
2.9206012389652987	0.8860452062691430	19.1709791912536573	T	T	T
4.3176308956800238	2.3384308127289457	21.2471705307211600	T	T	T
2.9137073215964193	0.8566465283561389	23.3419982255127145	T	T	T
2.8359139031792302	3.7602439029942856	19.1630214767349791	T	T	T
4.3322529614995835	5.1903633464841938	21.2264730395248442	T	T	T
2.8932761929247208	3.7593791152133074	23.3690676466314500	T	T	T
5.8217332091373866	0.9089203166884862	19.1951675317292114	T	T	T
7.2293557350581850	2.3630263788397201	21.2448843270352725	T	T	T
5.8004246090917642	0.8522818503936156	23.2690847894432515	T	T	T
5.7365057981952798	3.7605170433520811	19.1239690476089521	T	T	T
7.2364270146698013	5.1734015957441493	21.2046552973487117	T	T	T
5.7829043578064860	3.7592081316920285	23.3605888686123357	T	T	T
8.6950911603890084	0.9237219972394910	19.2134753900293767	T	T	T
10.1615847420140106	2.3627658804173048	21.2446005980288462	T	T	T
8.6964124455449703	0.8462540563970807	23.2391480344720627	T	T	T
8.6937843675827740	3.7666383203613996	19.1210147845888194	T	T	T
10.1550574441092287	5.1727512818429959	21.2039022473130778	T	T	T
8.6948613846002338	3.7558627060776533	23.3598717125472959	T	T	T
11.5692664590486469	0.9094480215412655	19.1952671229815834	T	T	T
13.0736168288057986	2.3390948809778562	21.2477395018515445	T	T	T
11.5917779088944233	0.8516229793796327	23.2689351504868540	T	T	T
11.6528761734414630	3.7609798315676128	19.1235994411345587	T	T	T
13.0585177482398809	5.1908182977154560	21.2262957999847757	T	T	T
11.6067679270228012	3.7584806679394394	23.3599797029166254	T	T	T
14.4715522161896768	0.8878805075273649	19.1716535495396840	T	T	T
15.9506167041645668	2.3232437035912095	21.2818538613813963	T	T	T
14.4777271431823156	0.8578205592366096	23.3430964937312204	T	T	T
14.5533873215072678	3.7623671411962549	19.1634052924272815	T	T	T
15.9410722144926886	5.2324610716170241	21.2858472628966773	T	T	T
14.4974829838053427	3.7608775232646092	23.3693313682234596	T	T	T

Oxide reference: ZnO(10-10)/fcc(100)_6x2/Au E_tot= -350.46856962 eV
D3-zero damping= -12.2849642 eV, D3-BJ damping= -12.6893737 eV
Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn
O Zn O Zn O Zn O Zn O Zn O Zn O Zn O

```
 1.0000000000000000
    17.3925102628200072    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7975034209400009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.1312880290811052
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2
Selective dynamics
Cartesian
  3.4784166234049381  5.7920814396558580  8.9451241821253618   F   F   F
  1.7391677333950526  2.8933297495539323  8.0000001838787966   F   F   F
  3.4784171936104840  3.5940765006679847  8.9451248436730744   F   F   F
  1.7391667701727282  0.6953248071507115  8.0000000000000000   F   F   F
  1.7391704735109343  5.7920813601461925 11.7805090714841079   F   F   F
  3.4784236360650502  2.8933296700442663 10.8353850732375427   F   F   F
  1.7391710437164798  3.5940764211583196 11.7805097330318205   F   F   F
  3.4784226728427257  0.6953247276410457 10.8353848893587461   F   F   F
  3.4783103401301250  5.6811175359448738 14.3570960327090660   T   T   T
  1.7391876964040704  2.8638484364981927 13.6462373927424121   T   T   T
  3.4786044220437184  3.6049943127015096 14.3867697374376231   T   T   T
  1.7392819143958118  0.7048710913685570 13.6581304909237353   T   T   T
  1.7391785925345444  5.4821103024613063 16.6830863296908625   T   T   T
  3.4785959266599988  2.7947703193823572 16.3532079619593134   T   T   T
  1.7392774449647910  3.5757693572784031 16.9014326507290598   T   T   T
  3.4784631525060070  0.6392850309488298 16.3263201177117914   T   T   T
  6.9569186759689394  5.7920814396558580  8.9451241821253618   F   F   F
  5.2176697859590542  2.8933297495539323  8.0000001838787966   F   F   F
  6.9569192461744853  3.5940765006679847  8.9451248436730744   F   F   F
  5.2176688227367300  0.6953248071507115  8.0000000000000000   F   F   F
  5.2176725260749359  5.7920813601461925 11.7805090714841079   F   F   F
  6.9569256886290516  2.8933296700442663 10.8353850732375427   F   F   F
  5.2176730962804818  3.5940764211583196 11.7805097330318205   F   F   F
  6.9569247254067266  0.6953247276410457 10.8353848893587461   F   F   F
  6.9568370978158285  5.6808012571815532 14.3572139594089485   T   T   T
  5.2175959765631106  2.8630844743391650 13.6459696749443467   T   T   T
  6.9570758449029295  3.6044675771137453 14.3865749733847483   T   T   T
  5.2177367916612090  0.7044008773142633 13.6581714785445225   T   T   T
  5.2175167886514542  5.4820562418894454 16.6829889954169239   T   T   T
  6.9570168107337178  2.7945969111591724 16.3529710487888984   T   T   T
  5.2178498733088299  3.5757001536884876 16.9012053525874997   T   T   T
  6.9569882173962716  0.6391033638920562 16.3261093843406151   T   T   T
 10.4354207285329412  5.7920814396558580  8.9451241821253618   F   F   F
  8.6961718385230533  2.8933297495539323  8.0000001838787966   F   F   F
 10.4354212987384862  3.5940765006679847  8.9451248436730744   F   F   F
  8.6961708753007301  0.6953248071507115  8.0000000000000000   F   F   F
  8.6961745786389386  5.7920813601461925 11.7805090714841079   F   F   F
 10.4354277411930525  2.8933296700442663 10.8353850732375427   F   F   F
  8.6961751488444818  3.5940764211583196 11.7805097330318205   F   F   F
 10.4354267779707275  0.6953247276410457 10.8353848893587461   F   F   F
 10.4356735961029017  5.6808255905371201 14.3571913206799646   T   T   T
  8.6962232868239919  2.8626656893306417 13.6458045428353056   T   T   T
 10.4354579753614587  3.6044725228993442 14.3865360736021568   T   T   T
  8.6962504576408612  0.7040800300174931 13.6583040178866923   T   T   T
  8.6963366159198259  5.4821475148257335 16.6824973718826790   T   T   T
 10.4356148949182792  2.7946267009671266 16.3529682429770595   T   T   T
  8.6962934910036545  3.5756853000406541 16.9007579292090249   T   T   T
 10.4356449013341788  0.6391581969125283 16.3260429810102394   T   T   T
 13.9139227810969430  5.7920814396558580  8.9451241821253618   F   F   F
 12.1746738910870569  2.8933297495539323  8.0000001838787966   F   F   F
 13.9139233513024898  3.5940765006679847  8.9451248436730744   F   F   F
 12.1746729278647319  0.6953248071507115  8.0000000000000000   F   F   F
 12.1746766312029404  5.7920813601461925 11.7805090714841079   F   F   F
 13.9139297937570561  2.8933296700442663 10.8353850732375427   F   F   F
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 12.1746772014084854  3.5940764211583196 11.7805097330318205   F   F   F
 13.9139288305347311  0.6953247276410457 10.8353848893587461   F   F   F
 13.9142511379344622  5.6811270160012972 14.3570578550566523   T   T   T
 12.1749251795130391  2.8630401473690235 13.6459392936664958   T   T   T
 13.9139072562154507  3.6050047752041721 14.3867186295049994   T   T   T
 12.1747950012768698  0.7043961505611179 13.6581622236082918   T   T   T
 12.1751379208679378  5.4820698016782075 16.6829340833180559   T   T   T
 13.9139744715411915  2.7948062934745077 16.3531918314645566   T   T   T
 12.1747250201310564  3.5757758869190610 16.9011501072972834   T   T   T
 13.9141649278670911  0.6393270620463782 16.3262848741654629   T   T   T
 17.3924248336609466  5.7920814396558580  8.9451241821253618   F   F   F
 15.6531759436510569  2.8933297495539323  8.0000001838787966   F   F   F
 17.3924254038664898  3.5940765006679847  8.9451248436730744   F   F   F
 15.6531749804287319  0.6953248071507115  8.0000000000000000   F   F   F
 15.6531786837669387  5.7920813601461925 11.7805090714841079   F   F   F
 17.3924318463210561  2.8933296700442663 10.8353850732375427   F   F   F
 15.6531792539724854  3.5940764211583196 11.7805097330318205   F   F   F
 17.3924308830987293  0.6953247276410457 10.8353848893587461   F   F   F
 17.3925624827955083  5.6815155431502866 14.3571191884629759   T   T   T
 15.6533376626679672  2.8638641694597795 13.6462436806398806   T   T   T
 17.3925154404867293  3.6053056644020507 14.3868236627548569   T   T   T
 15.6532845702944297  0.7048789906537807 13.6581348905127395   T   T   T
 15.6534547690148624  5.4821352222742616 16.6830949954903680   T   T   T
 17.3925189461279182  2.7948390275714732 16.3532533259638271   T   T   T
 15.6533216743228483  3.5758393139294178 16.9013618328973187   T   T   T
 17.3925761400938050  0.6394502408752454 16.3263725167705189   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_6x2/Au E_tot= -120.04081143 eV
 D3-zero damping= -14.7699681 eV, D3-BJ damping= -14.9065456 eV
Au
 1.0000000000000000
    17.3925102628200072    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7975034209400009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9359299014895974
  36
Cartesian
  0.0000000255786493 -0.0000000000000001  7.8927337513832043
  1.4493758552349991  1.4493758552350002  9.9738292057041420
  0.0000000255786493  0.0000000000000000 12.0528014656305213
  0.0000000255786493  2.8987517104700005  7.8927337513832043
  1.4493758552349991  4.3481275657050018  9.9738292057041420
  0.0000000255786493  2.8987517104700005 12.0528014656305213
  2.8987517104699982  0.0000000000000000  7.8927337961858868
  4.3481275252601765  1.4493758552350002  9.9738292356406362
  2.8987517104699982  0.0000000000000000 12.0528015113080773
  2.8987517104699982  2.8987517104700005  7.8927337961858868
  4.3481275252601765  4.3481275657050018  9.9738292356406362
  2.8987517104699982  2.8987517104700005 12.0528015113080773
  5.7975033953613542 -0.0000000000000000  7.8927337703870757
  7.2468792792333181  1.4493758552350002  9.9738291611216141
  5.7975033953613542  0.0000000000000000 12.0528014356940218
  5.7975033953613542  2.8987517104700005  7.8927337703870757
  7.2468792792333181  4.3481275657050018  9.9738291462554240
  5.7975033953613542  2.8987517104700005 12.0528014356940218
  8.6962551314100036  0.0000000000000000  7.8927336449418179
 10.1456310015111821  1.4493758552350002  9.9738290706413721
  8.6962551314100036 -0.0000000000000000 12.0528014912091610
  8.6962551314100036  2.8987517104700005  7.8927336449418179
 10.1456310015111821  4.3481275657050018  9.9738290706413721
  8.6962551314100036  2.8987517104700005 12.0528014912091610
 11.5950068418800001 -0.0000000000000000  7.8927336449418179
 13.0443826940566865  1.4493758552350002  9.9738291611216141
 11.5950068418800001  0.0000000000000000 12.0528014912091610
```

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 11.5950068418800001  2.8987517104700005  7.8927336449418179
 13.0443827078274683  4.3481275657050018  9.9738291611216141
 11.5950068418800001  2.8987517104700005 12.0528014912091610
 14.4937585523500037 -0.0000000000000000  7.8927337566162974
 15.9431344032271447  1.4493758552350002  9.9738292057041420
 14.4937585523500037  0.0000000000000000 12.0528014612726615
 14.4937585523500037  2.8987517104700005  7.8927337566162974
 15.9431344032271447  4.3481275657050018  9.9738292057041420
 14.4937585523500037  2.8987517104700005 12.0528014612726615

Interface: ZnO(10-10)/fcc(100)_6x2/Ag E_tot= -459.13148828 eV
 D3-zero damping= -29.2502053 eV, D3-BJ damping= -30.8089954 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Ag
 1.0000000000000000
    17.2831623117000035    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7610541039000012    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.3241942887299736
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2  36
Selective dynamics
Cartesian
  3.4565475702801476  5.7556662109984709  8.9451241821253618   F   F   F
  1.7282334619513668  2.8751391792884893  8.0000001838787966   F   F   F
  3.4565481369007705  3.5714802856548644  8.9451248436730744   F   F   F
  1.7282325047848899  0.6909532505510081  8.0000000000000000   F   F   F
  1.7282361848399448  5.7556661319886882 11.7805090714841079   F   F   F
  3.4565545388511656  2.8751391002787066 10.8353850732375427   F   F   F
  1.7282367514605672  3.5714802066450821 11.7805097330318205   F   F   F
  3.4565535816846884  0.6909531715412253 10.8353848893587461   F   F   F
  3.4465444876275031  5.6301834131245858 14.3737041207755674   T   T   T
  1.7280538503121927  2.8068183715174864 13.6253020619092471   T   T   T
  3.4562408063422660  3.5684321230822933 14.4085231008966872   T   T   T
  1.7242244551171599  0.6938066029448384 13.6619951286350325   T   T   T
  1.7053363328166169  5.6290433067588479 16.9313991576736527   T   T   T
  3.4618068454157456  2.7892414507541372 16.2999932520069066   T   T   T
  1.7374650580871818  3.6425353862506582 16.9453585103948576   T   T   T
  3.4422585979627551  0.7119635217420841 16.2847651505400677   T   T   T
  6.9131800326201480  5.7556662109984709  8.9451241821253618   F   F   F
  5.1848659242913682  2.8751391792884893  8.0000001838787966   F   F   F
  6.9131805992407722  3.5714802856548644  8.9451248436730744   F   F   F
  5.1848649671248914  0.6909532505510081  8.0000000000000000   F   F   F
  5.1848686471799459  5.7556661319886882 11.7805090714841079   F   F   F
  6.9131870011911669  2.8751391002787066 10.8353850732375427   F   F   F
  5.1848692138005692  3.5714802066450821 11.7805097330318205   F   F   F
  6.9131860440246893  0.6909531715412253 10.8353848893587461   F   F   F
  6.9070230501243790  5.6237312889905002 14.3837056301362765   T   T   T
  5.1887149193997679  2.8038817665860076 13.6249781210257659   T   T   T
  6.9139470509580843  3.5612602663901920 14.4101616291133450   T   T   T
  5.1804094994105689  0.6876826277924836 13.6673228735208987   T   T   T
  5.1459569769058575  5.6028557906838570 16.8947408083397406   T   T   T
  6.9189382806553823  2.7726166512263939 16.3134814657810026   T   T   T
  5.1926851524768871  3.6174487497592782 16.9119254393078435   T   T   T
  6.9026205096924347  0.6945274157003306 16.2997357772626330   T   T   T
 10.3698124949601489  5.7556662109984709  8.9451241821253618   F   F   F
  8.6414983866313673  2.8751391792884893  8.0000001838787966   F   F   F
 10.3698130615807731  3.5714802856548644  8.9451248436730744   F   F   F
  8.6414974294648914  0.6909532505510081  8.0000000000000000   F   F   F
  8.6415011095199485  5.7556661319886882 11.7805090714841079   F   F   F
 10.3698194635311687  2.8751391002787066 10.8353850732375427   F   F   F
  8.6415016761405692  3.5714802066450821 11.7805097330318205   F   F   F
 10.3698185063646910  0.6909531715412253 10.8353848893587461   F   F   F
```

10.3758361207031111	5.6236703042517542	14.3832318234219994	T	T	T
8.6406104952574179	2.8009721678295962	13.6246293772965199	T	T	T
10.3681183363294593	3.5612051577440118	14.4097862157811676	T	T	T
8.6413612799304040	0.6832695699606530	13.6711982090572501	T	T	T
8.6424711090216046	5.6039015956807994	16.8735953151598004	T	T	T
10.3645271633684022	2.7728642069463842	16.3131136223431419	T	T	T
8.6409837860671068	3.6122326816548713	16.9039120452235103	T	T	T
10.3810101536632491	0.6949431567426609	16.2993998722630167	T	T	T
13.8264449573001507	5.7556662109984709	8.9451241821253618	F	F	F
12.0981308489713708	2.8751391792884893	8.0000001838787966	F	F	F
13.8264455239207749	3.5714802856548644	8.9451248436730744	F	F	F
12.0981298918048932	0.6909532505510081	8.0000000000000000	F	F	F
12.0981335718599503	5.7556661319886882	11.7805090714841079	F	F	F
13.8264519258711704	2.8751391002787066	10.8353850732375427	F	F	F
12.0981341384805727	3.5714802066450821	11.7805097330318205	F	F	F
13.8264509687046946	0.6909531715412253	10.8353848893587461	F	F	F
13.8363151139513061	5.6300191065067438	14.3740005875323096	T	T	T
12.0933963670500226	2.8037482823710413	13.6248604809380449	T	T	T
13.8259466017879866	3.5682943990273350	14.4087061055627412	T	T	T
12.1023195415561293	0.6876973456109430	13.6670719882156337	T	T	T
12.1374511727339005	5.6032362096559725	16.8950151539945246	T	T	T
13.8213086866523458	2.7895068128990297	16.3001380565839042	T	T	T
12.0902220145412169	3.6174606316651752	16.9125921296393003	T	T	T
13.8402936787670772	0.7121895952813428	16.2848389943451544	T	T	T
17.2830774196401542	5.7556662109984709	8.9451241821253618	F	F	F
15.5547633113113708	2.8751391792884893	8.0000001838787966	F	F	F
17.2830779862607748	3.5714802856548644	8.9451248436730744	F	F	F
15.5547623541448932	0.6909532505510081	8.0000000000000000	F	F	F
15.5547660341999485	5.7556661319886882	11.7805090714841079	F	F	F
17.2830843882111722	2.8751391002787066	10.8353850732375427	F	F	F
15.5547666008205727	3.5714802066450821	11.7805097330318205	F	F	F
17.2830834310446910	0.6909531715412253	10.8353848893587461	F	F	F
17.2823898852489322	5.6327189886363742	14.3751089207489677	T	T	T
15.5540968848022008	2.8066839904461069	13.6254367733733446	T	T	T
17.2828209846818837	3.5713031784805480	14.4167437478019540	T	T	T
15.5581287053532336	0.6939276939669419	13.6617110249686515	T	T	T
15.5767477934079057	5.6297157471177899	16.9339717780573693	T	T	T
17.2829623062430002	2.8056046309433791	16.3085693350288601	T	T	T
15.5457976230313033	3.6433595921687028	16.9467158081688041	T	T	T
17.2829969870062108	0.7244653021737323	16.2791558640049452	T	T	T
-0.0063993346145748	1.0628581749542401	19.1042678305732245	T	T	T
1.4337747432593111	2.5042838867335173	21.1517701100161872	T	T	T
-0.0074900702702766	1.0559362714870602	23.2126752559242959	T	T	T
-0.0067441112424403	3.9406548632867771	19.1220125472114191	T	T	T
1.4369567702489607	5.3875183943412503	21.1437486640477168	T	T	T
-0.0076096331037223	3.9394239160032187	23.1999545481561498	T	T	T
2.9270000037771471	1.0769812114011121	19.1179701860620312	T	T	T
4.3073176795841377	2.5382755207836403	21.1923926014723847	T	T	T
2.8575196233885758	1.0706433410065888	23.2221381644460436	T	T	T
2.8748338360884795	3.9462556312416548	19.1207059450751160	T	T	T
4.3142943544198227	5.3982926638449173	21.1745888809110774	T	T	T
2.8552261901062019	3.9561919019933236	23.2262989516169078	T	T	T
5.8044965232395089	1.1384212962496520	19.1722045121546536	T	T	T
7.1878470779112567	2.5819381393894982	21.2447153441992533	T	T	T
5.7346408220330334	1.1011737425965922	23.2436817546373220	T	T	T
5.7528457020891954	3.9847158898056176	19.1609937591227606	T	T	T
7.1931773606476295	5.4210474702442859	21.2093513485863312	T	T	T
5.7345470640870211	3.9911278356161723	23.2808020907868567	T	T	T
8.6329723450544762	1.1722453915837800	19.2067470329968550	T	T	T
10.0777493379105501	2.5816806074979253	21.2431329682287213	T	T	T
8.6331547417749004	1.1179384606685672	23.2545327002058890	T	T	T
8.6350284816935439	4.0047344382301215	19.1815401366325879	T	T	T
10.0738151509937151	5.4219397609216173	21.2077406268699242	T	T	T

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  8.6356973007044289  4.0087951721696733 23.3026810998758940   T   T   T
 11.4635476070109235  1.1378603862697962 19.1715465273489905   T   T   T
 12.9602374250318206  2.5374713436048548 21.1898551324009929   T   T   T
 11.5311743011234942  1.1012596631025637 23.2408812096013158   T   T   T
 11.5159309207706535  3.9848796248944769 19.1603166455469172   T   T   T
 12.9546847517898698  5.3986194839232349 21.1733798750505287   T   T   T
 11.5349288168932649  3.9919132774198927 23.2778290925678135   T   T   T
 14.3438562251925692  1.0759264075291282 19.1181994847188967   T   T   T
 15.8363693926882441  2.5037813793581325 21.1514372203995329   T   T   T
 14.4091541455575491  1.0700481067926897 23.2203766581607667   T   T   T
 14.3949142498716807  3.9460095685415220 19.1206993684932520   T   T   T
 15.8344632892240469  5.3872641715095382 21.1436810433031859   T   T   T
 14.4126367744701493  3.9555385767446660 23.2233721805594300   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_6x2/Ag E_tot= -351.81838756 eV
 D3-zero damping= -12.3571273 eV, D3-BJ damping= -12.827013 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
    17.2831623117000035    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7610541039000012    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.1312880290811052
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2
Selective dynamics
Cartesian
  3.4565475702801476  5.7556662109984709  8.9451241821253618   F   F   F
  1.7282334619513668  2.8751391792884893  8.0000001838787966   F   F   F
  3.4565481369007705  3.5714802856548644  8.9451248436730744   F   F   F
  1.7282325047848899  0.6909532505510081  8.0000000000000000   F   F   F
  1.7282361848399448  5.7556661319886882 11.7805090714841079   F   F   F
  3.4565545388511656  2.8751391002787066 10.8353850732375427   F   F   F
  1.7282367514605672  3.5714802066450821 11.7805097330318205   F   F   F
  3.4565535816846884  0.6909531715412253 10.8353848893587461   F   F   F
  3.4566522825200838  5.6436099573740757 14.3668417461522164   T   T   T
  1.7283244852183781  2.8410382288573799 13.6482563028776767   T   T   T
  3.4565132753979650  3.5808269494688658 14.4040022066794844   T   T   T
  1.7283193758290589  0.7022028539291413 13.6595734531779502   T   T   T
  1.7282779857460351  5.4493427002118953 16.7055941440931832   T   T   T
  3.4566468779292787  2.7734640161702293 16.3725882938447604   T   T   T
  1.7280608938183790  3.5510384572746974 16.9377034940554090   T   T   T
  3.4566131758881662  0.6410846248985005 16.3363003885785965   T   T   T
  6.9131800326201480  5.7556662109984709  8.9451241821253618   F   F   F
  5.1848659242913682  2.8751391792884893  8.0000001838787966   F   F   F
  6.9131805992407722  3.5714802856548644  8.9451248436730744   F   F   F
  5.1848649671248914  0.6909532505510081  8.0000000000000000   F   F   F
  5.1848686471799459  5.7556661319886882 11.7805090714841079   F   F   F
  6.9131870011911669  2.8751391002787066 10.8353850732375427   F   F   F
  5.1848692138005692  3.5714802066450821 11.7805097330318205   F   F   F
  6.9131860440246893  0.6909531715412253 10.8353848893587461   F   F   F
  6.9133145823376649  5.6430884759253370 14.3669203950169457   T   T   T
  5.1847251048620731  2.8400826581836731 13.6480025187614853   T   T   T
  6.9130708855643563  3.5800786977613055 14.4035236469074128   T   T   T
  5.1847791380304580  0.7016585860568606 13.6594777736372901   T   T   T
  5.1850143712454946  5.4482863096644714 16.7055850866219622   T   T   T
  6.9132714026613531  2.7727610233233655 16.3722679509302225   T   T   T
  5.1847498728304577  3.5502264563730868 16.9377644625024040   T   T   T
  6.9130836087003527  0.6405246128751291 16.3362427711740104   T   T   T
 10.3698124949601489  5.7556662109984709  8.9451241821253618   F   F   F
  8.6414983866313673  2.8751391792884893  8.0000001838787966   F   F   F
 10.3698130615807731  3.5714802856548644  8.9451248436730744   F   F   F
  8.6414974294648914  0.6909532505510081  8.0000000000000000   F   F   F
```

```
  8.6415011095199485  5.7556661319886882 11.7805090714841079   F   F   F
 10.3698194635311687  2.8751391002787066 10.8353850732375427   F   F   F
  8.6415016761405692  3.5714802066450821 11.7805097330318205   F   F   F
 10.3698185063646910  0.6909531715412253 10.8353848893587461   F   F   F
 10.3699272229706043  5.6431282317583653 14.3669724780059429   T   T   T
  8.6415991395158063  2.8397350768405594 13.6480291649462657   T   T   T
 10.3700238294061968  3.5800938159903293 14.4035172933486599   T   T   T
  8.6415361882751096  0.7013817984603374 13.6594726604297048   T   T   T
  8.6415650135055966  5.4478352275729236 16.7053151361875010   T   T   T
 10.3699175767480902  2.7727170925636750 16.3721846272033673   T   T   T
  8.6415123603020838  3.5502231864676039 16.9372022673498854   T   T   T
 10.3699124665226865  0.6405367703957844 16.3362757220296757   T   T   T
 13.8264449573001507  5.7556662109984709  8.9451241821253618   F   F   F
 12.0981308489713708  2.8751391792884893  8.0000001838787966   F   F   F
 13.8264455239207749  3.5714802856548644  8.9451248436730744   F   F   F
 12.0981298918048932  0.6909532505510081  8.0000000000000000   F   F   F
 12.0981335718599503  5.7556661319886882 11.7805090714841079   F   F   F
 13.8264519258711704  2.8751391002787066 10.8353850732375427   F   F   F
 12.0981341384805727  3.5714802066450821 11.7805097330318205   F   F   F
 13.8264509687046946  0.6909531715412253 10.8353848893587461   F   F   F
 13.8264663080769914  5.6435737228462379 14.3668959098645654   T   T   T
 12.0984104979823197  2.8401211305646985 13.6479972729993140   T   T   T
 13.8266457573296915  3.5807851833307960 14.4039678340271795   T   T   T
 12.0983319717831392  0.7016440974805114 13.6594490184969075   T   T   T
 12.0981241104625230  5.4482979234582558 16.7056405327759734   T   T   T
 13.8264178655836520  2.7734414172684483 16.3725796349450867   T   T   T
 12.0983348997020990  3.5502852403436873 16.9377450861013052   T   T   T
 13.8265331915461278  0.6410816903178338 16.3363200721702064   T   T   T
 17.2830774196401542  5.7556662109984709  8.9451241821253618   F   F   F
 15.5547633113113708  2.8751391792884893  8.0000001838787966   F   F   F
 17.2830779862607748  3.5714802856548644  8.9451248436730744   F   F   F
 15.5547623541448932  0.6909532505510081  8.0000000000000000   F   F   F
 15.5547660341999485  5.7556661319886882 11.7805090714841079   F   F   F
 17.2830843882111722  2.8751391002787066 10.8353850732375427   F   F   F
 15.5547666008205727  3.5714802066450821 11.7805097330318205   F   F   F
 17.2830834310446910  0.6909531715412253 10.8353848893587461   F   F   F
 17.2831256385980012  5.6441028929263766 14.3665516785131953   T   T   T
 15.5547850776933370  2.8410138899831083 13.6482775949841066   T   T   T
 17.2831737313517628  3.5813503431559015 14.4038831795893891   T   T   T
 15.5548294222047883  0.7021873583118842 13.6595606655967945   T   T   T
 15.5548362458540481  5.4493212257197960 16.7056183422696662   T   T   T
 17.2830647395830717  2.7739652339988292 16.3721320850919163   T   T   T
 15.5551878269926149  3.5510483876307783 16.9376986356345611   T   T   T
 17.2831907500941284  0.6416927515094545 16.3361550532432318   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_6x2/Ag E_tot= -98.04341515 eV
 D3-zero damping= -10.8013157 eV, D3-BJ damping= -13.602698 eV
Ag
 1.0000000000000000
    17.2831623117000035    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7610541039000012    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9359299014895974
  36
Cartesian
  0.0000000000000000  0.0000000000000000  7.9182351364057473
  1.4402635259749992  1.4402635259750003  9.9733953365639607
 -0.0000000000000000 -0.0000000000000000 12.0277339046602343
 -0.0000000000000000  2.8805270519500006  7.9182351364057473
  1.4402635259749992  4.3207905779250009  9.9733953365639607
  0.0000000000000000  2.8805270519500006 12.0277339046602343
  2.8805270525730275 -0.0000000000000000  7.9182351364057473
  4.3207905785480287  1.4402635259750003  9.9733953365639607
  2.8805270525730275  0.0000000000000000 12.0277339046602343
```

```
  2.8805270525730275  2.8805270519500006  7.9182351364057473
  4.3207905785480287  4.3207905779250009  9.9733953365639607
  2.8805270525730275  2.8805270519500006 12.0277339046602343
  5.7610541566001663  0.0000000000000000  7.9182350843286082
  7.2013176819521432  1.4402635259750003  9.9733953365639607
  5.7610541566001663  0.0000000000000000 12.0277339567373698
  5.7610541566001663  2.8805270519500006  7.9182350843286082
  7.2013176819521432  4.3207905779250009  9.9733953365639607
  5.7610541566001663  2.8805270519500006 12.0277339567373698
  8.6415812079271372  0.0000000000000000  7.9182350843286082
 10.0818446812019644  1.4402635259750003  9.9733953365639607
  8.6415812079271372 -0.0000000000000000 12.0277339567373698
  8.6415812079271372  2.8805270519500006  7.9182350843286082
 10.0818446812019644  4.3207905779250009  9.9733953365639607
  8.6415812079271372  2.8805270519500006 12.0277339567373698
 11.5221081550998310  0.0000000000000000  7.9182351364057473
 12.9623716810748348  1.4402635259750003  9.9733953365639607
 11.5221081550998310  0.0000000000000000 12.0277339046602343
 11.5221081550998310  2.8805270519500006  7.9182351364057473
 12.9623716810748348  4.3207905779250009  9.9733953365639607
 11.5221081550998310  2.8805270519500006 12.0277339046602343
 14.4026352597500029  0.0000000000000000  7.9182351364057473
 15.8428987857250014  1.4402635259750003  9.9733953816518621
 14.4026352070498334 -0.0000000000000000 12.0277339567373698
 14.4026352597500029  2.8805270519500006  7.9182351364057473
 15.8428987857250014  4.3207905779250009  9.9733953816518621
 14.4026352070498334  2.8805270519500006 12.0277339567373698

Interface: ZnO(10-10)/fcc(100)_6x2/Cu E_tot= -493.8153299 eV
 D3-zero damping= -28.8185116 eV, D3-BJ damping= -33.3279754 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Cu
 1.0000000000000000
    15.1426178203800053    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.0475392734600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.3241942887299736
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2  36
Selective dynamics
Cartesian
  3.0284491860197655  5.0428186788376976  8.9451241821253618   F   F   F
  1.5141892639060488  2.5190490598409605  8.0000001838787966   F   F   F
  3.0284496824636098  3.1291473194163189  8.9451248436730744   F   F   F
  1.5141884252860156  0.6053776974460434  8.0000000000000000   F   F   F
  1.5141916495609631  5.0428186096133896 11.7805090714841079   F   F   F
  3.0284552915232479  2.5190489906166529 10.8353850732375427   F   F   F
  1.5141921460048071  3.1291472501920117 11.7805097330318205   F   F   F
  3.0284544529032145  0.6053776282217357 10.8353848893587461   F   F   F
  3.0181282233489628  5.1063483360797584 14.8118534546477090   T   T   T
  1.5153648801781325  2.5655134887830759 13.7028824964357376   T   T   T
  3.0243597152812183  3.1299438466947391 14.8421072041958571   T   T   T
  1.5134468359427138  0.6019389885659565 13.6735359356813220   T   T   T
  1.4565049756087054  5.1882561155746609 17.8935436914592039   T   T   T
  2.9972247548273145  2.6052834208187012 16.7440679227466163   T   T   T
  1.4990311464548214  3.1834083785058680 17.9138679155919682   T   T   T
  2.9664056168639616  0.6315710546050012 16.6863930527012840   T   T   T
  6.0569727500957660  5.0428186788376976  8.9451241821253618   F   F   F
  4.5427128279820499  2.5190490598409605  8.0000001838787966   F   F   F
  6.0569732465396111  3.1291473194163189  8.9451248436730744   F   F   F
  4.5427119893620169  0.6053776974460434  8.0000000000000000   F   F   F
  4.5427152136369644  5.0428186096133896 11.7805090714841079   F   F   F
  6.0569788555992492  2.5190489906166529 10.8353850732375427   F   F   F
```

4.5427157100808095	3.1291472501920117	11.7805097330318205	F	F	F
6.0569780169792153	0.6053776282217357	10.8353848893587461	F	F	F
6.0482728274488560	5.1001512526464472	14.8147852884507589	T	T	T
4.5379666846124591	2.5623383262101216	13.7059972465447153	T	T	T
6.0563099190209497	3.1220276490094001	14.8289362138396612	T	T	T
4.5351541416840924	0.5954020963449671	13.6841023247294427	T	T	T
4.4529992919271004	5.1418797326072232	17.8463004264868061	T	T	T
6.0419541631858822	2.5836263857978587	16.7288041621385659	T	T	T
4.5379017306556051	3.1531665269019831	17.8449741502796080	T	T	T
6.0124748900862324	0.6056076964098198	16.7050991571297054	T	T	T
9.0854963141717668	5.0428186788376976	8.9451241821253618	F	F	F
7.5712363920580499	2.5190490598409605	8.0000001838787966	F	F	F
9.0854968106156111	3.1291473194163189	8.9451248436730744	F	F	F
7.5712355534380169	0.6053776974460434	8.0000000000000000	F	F	F
7.5712387777129662	5.0428186096133896	11.7805090714841079	F	F	F
9.0855024196752510	2.5190489906166529	10.8353850732375427	F	F	F
7.5712392741568086	3.1291472501920117	11.7805097330318205	F	F	F
9.0855015810552171	0.6053776282217357	10.8353848893587461	F	F	F
9.0951932093613355	5.1000695871878570	14.8150954997904538	T	T	T
7.5721291453402833	2.5584091339091000	13.7024332799831416	T	T	T
9.0876253272998540	3.1221022126559688	14.8290143351072423	T	T	T
7.5717092433072635	0.5896219085563176	13.6920388438049638	T	T	T
7.5719218504519255	5.1019497499881208	17.7687932168294225	T	T	T
9.1025369021967730	2.5838886105540033	16.7290667072005981	T	T	T
7.5721319769212467	3.1229919083351381	17.8313316431856954	T	T	T
9.1314927567630413	0.6055758594750802	16.7054568512470283	T	T	T
12.1140198782477686	5.0428186788376976	8.9451241821253618	F	F	F
10.5997599561340525	2.5190490598409605	8.0000001838787966	F	F	F
12.1140203746916146	3.1291473194163189	8.9451248436730744	F	F	F
10.5997591175140187	0.6053776974460434	8.0000000000000000	F	F	F
10.5997623417889670	5.0428186096133896	11.7805090714841079	F	F	F
12.1140259837512527	2.5190489906166529	10.8353850732375427	F	F	F
10.5997628382328113	3.1291472501920117	11.7805097330318205	F	F	F
12.1140251451312189	0.6053776282217357	10.8353848893587461	F	F	F
12.1250162337897489	5.1066614976788296	14.8118738845589970	T	T	T
10.6061699239134217	2.5624584126934575	13.7060272240795182	T	T	T
12.1195371035825552	3.1302851269270100	14.8421979131505530	T	T	T
10.6081933301864648	0.5956530787029372	13.6840388027027142	T	T	T
10.6913834632541800	5.1423829122454565	17.8462934249151353	T	T	T
12.1478600255403872	2.6059210312505701	16.7443249084195536	T	T	T
10.6066779541177230	3.1535673996522333	17.8447812566552066	T	T	T
12.1777646542467881	0.6321508330412696	16.6863787465082254	T	T	T
15.1425434423237721	5.0428186788376976	8.9451241821253618	F	F	F
13.6282835202100525	2.5190490598409605	8.0000001838787966	F	F	F
15.1425439387676146	3.1291473194163189	8.9451248436730744	F	F	F
13.6282826815900187	0.6053776974460434	8.0000000000000000	F	F	F
13.6282859058649670	5.0428186096133896	11.7805090714841079	F	F	F
15.1425495478272527	2.5190489906166529	10.8353850732375427	F	F	F
13.6282864023088113	3.1291472501920117	11.7805097330318205	F	F	F
15.1425487092072171	0.6053776282217357	10.8353848893587461	F	F	F
15.1430402249603446	5.1066463185707676	14.7969659472762256	T	T	T
13.6283675325050151	2.5654593363445395	13.7028548323389732	T	T	T
15.1432200556263883	3.1325994721830126	14.8358486094543949	T	T	T
13.6299049686186962	0.6019500159077712	13.6734499108234324	T	T	T
13.6873774979975007	5.1885029396725182	17.8932528056969211	T	T	T
15.1443458197400087	2.6117737621697068	16.7321615822827070	T	T	T
13.6464749951399771	3.1834176771432077	17.9137834688973747	T	T	T
15.1434988685717737	0.6433473096081526	16.6608292112266128	T	T	T
0.0004577184994618	0.7944732814818268	19.8972275974657400	T	T	T
1.2568726679412501	2.1027414970085800	21.6279008814031819	T	T	T
0.0003262486540074	0.8135164028325836	23.3989228494655279	T	T	T
0.0003246347477246	3.3073355819860573	19.7266235263161818	T	T	T
1.2632600683571122	4.5812939429325628	21.6293994242426777	T	T	T

```
  0.0003023605079070  3.3376255573146385 23.4256755102685155   T   T   T
  2.6065597458285592  0.8338035647450582 19.9375099041057418   T   T   T
  3.7716358141501782  2.1701613163684597 21.6880100354909757   T   T   T
  2.5057696319947738  0.8442416202489593 23.4200042426547306   T   T   T
  2.4857363042346217  3.3461946860254073 19.7736131898879215   T   T   T
  3.7891656667736262  4.6210441353161986 21.6833327141808105   T   T   T
  2.5029762876734010  3.3688103979800612 23.4601997966525779   T   T   T
  5.1014840009277886  0.9251042475156217 20.0213439525073120   T   T   T
  6.3039820736507073  2.2250173274887954 21.7277771554246470   T   T   T
  5.0342389928180022  0.8979880867226658 23.4492834474000773   T   T   T
  5.0020681787692665  3.4268624550390134 19.8066713242509458   T   T   T
  6.3123189645202933  4.6565704744519021 21.7059092645582403   T   T   T
  5.0316387279189563  3.4229513902858089 23.5101809748459374   T   T   T
  7.5717029136386893  0.9494421214398315 20.0345052684680098   T   T   T
  8.8395210796639283  2.2249447464850824 21.7277052110433750   T   T   T
  7.5717791611564262  0.9178367173035684 23.4594042760854578   T   T   T
  7.5719379219102541  3.4477615286758714 19.8197259177483929   T   T   T
  8.8311831045955635  4.6565372097287705 21.7058937706032644   T   T   T
  7.5717838064333405  3.4437884613244214 23.5283986721867571   T   T   T
 10.0418538038021889  0.9250176119419437 20.0213369713207889   T   T   T
 11.3718043623691045  2.1699954200999341 21.6878472396293773   T   T   T
 10.1092171473026973  0.8979324621847706 23.4492878019435089   T   T   T
 10.1416778398708090  3.4267809543263255 19.8065383773995016   T   T   T
 11.3542701576715341  4.6209472291220521 21.6832238741418166   T   T   T
 10.1118572344569344  3.4228980659589738 23.5101527772488765   T   T   T
 12.5367993878733213  0.8334969883800517 19.9372144166239451   T   T   T
 13.8863860273730619  2.1025483229205628 21.6278135496762189   T   T   T
 12.6375083683401392  0.8441137182104246 23.4200393733546797   T   T   T
 12.6577776577835923  3.3458734943995250 19.7732824558338010   T   T   T
 13.8800096174557321  4.5812174934276015 21.6293300718571579   T   T   T
 12.6403290578116039  3.3687016100638387 23.4601359826248448   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_6x2/Cu E_tot= -353.44356322 eV
 D3-zero damping= -13.942947 eV, D3-BJ damping= -15.7603641 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
    15.1426178203800053    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.0475392734600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.1312880290811052
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2
Selective dynamics
Cartesian
  3.0284491860197655  5.0428186788376976  8.9451241821253618   F   F   F
  1.5141892639060488  2.5190490598409605  8.0000001838787966   F   F   F
  3.0284496824636098  3.1291473194163189  8.9451248436730744   F   F   F
  1.5141884252860156  0.6053776974460434  8.0000000000000000   F   F   F
  1.5141916495609631  5.0428186096133896 11.7805090714841079   F   F   F
  3.0284552915232479  2.5190489906166529 10.8353850732375427   F   F   F
  1.5141921460048071  3.1291472501920117 11.7805097330318205   F   F   F
  3.0284544529032145  0.6053776282217357 10.8353848893587461   F   F   F
  3.0277977729069794  5.0914213964397863 14.7725977781772073   T   T   T
  1.5142786995703319  2.5798948261987937 13.7217576652416771   T   T   T
  3.0286089787825716  3.1227012672913586 14.8609548568825645   T   T   T
  1.5137840807337322  0.6114286393812535 13.6739197262307943   T   T   T
  1.5142210324018166  4.8851420902381282 17.5775952010492063   T   T   T
  3.0277261243652966  2.5809505917004363 16.8173491931505588   T   T   T
  1.5144310345884633  3.0667158019261453 17.9335904745333927   T   T   T
  3.0286445148510444  0.6237495659983537 16.6799181497431555   T   T   T
  6.0569727500957660  5.0428186788376976  8.9451241821253618   F   F   F
  4.5427128279820499  2.5190490598409605  8.0000001838787966   F   F   F
```

6.0569732465396111	3.1291473194163189	8.9451248436730744	F	F	F
4.5427119893620169	0.6053776974460434	8.0000000000000000	F	F	F
4.5427152136369644	5.0428186096133896	11.7805090714841079	F	F	F
6.0569788555992492	2.5190489906166529	10.8353850732375427	F	F	F
4.5427157100808095	3.1291472501920117	11.7805097330318205	F	F	F
6.0569780169792153	0.6053776282217357	10.8353848893587461	F	F	F
6.0565400859590959	5.0900330292780049	14.7713562235770848	T	T	T
4.5424388085606946	2.5793818204936421	13.7211420962459876	T	T	T
6.0571984057574344	3.1214805200532720	14.8594063643736352	T	T	T
4.5420652004272863	0.6108072578492486	13.6738217984280475	T	T	T
4.5427886212087163	4.8827328462600592	17.5764738537308460	T	T	T
6.0562542598804230	2.5788992283299241	16.8153049662874956	T	T	T
4.5430098412168576	3.0642513639425184	17.9315433363543946	T	T	T
6.0570443782122760	0.6217179231285910	16.6787010522169012	T	T	T
9.0854963141717668	5.0428186788376976	8.9451241821253618	F	F	F
7.5712363920580499	2.5190490598409605	8.0000001838787966	F	F	F
9.0854968106156111	3.1291473194163189	8.9451248436730744	F	F	F
7.5712355534380169	0.6053776974460434	8.0000000000000000	F	F	F
7.5712387777129662	5.0428186096133896	11.7805090714841079	F	F	F
9.0855024196752510	2.5190489906166529	10.8353850732375427	F	F	F
7.5712392741568086	3.1291472501920117	11.7805097330318205	F	F	F
9.0855015810552171	0.6053776282217357	10.8353848893587461	F	F	F
9.0865078845237495	5.0902539010826082	14.7716388116745119	T	T	T
7.5715355279198251	2.5782523146559657	13.7207812938158060	T	T	T
9.0857788962919983	3.1216499109107514	14.8595487640454778	T	T	T
7.5715620699060864	0.6097606576071185	13.6739351103231854	T	T	T
7.5715798262235774	4.8812951078943865	17.5748672539492361	T	T	T
9.0866118325903180	2.5790656083868044	16.8154129189826129	T	T	T
7.5713595309907573	3.0627869185518874	17.9291302752775010	T	T	T
9.0861197750168046	0.6218770453797049	16.6789876126926195	T	T	T
12.1140198782477686	5.0428186788376976	8.9451241821253618	F	F	F
10.5997599561340525	2.5190490598409605	8.0000001838787966	F	F	F
12.1140203746916146	3.1291473194163189	8.9451248436730744	F	F	F
10.5997591175140187	0.6053776974460434	8.0000000000000000	F	F	F
10.5997623417889670	5.0428186096133896	11.7805090714841079	F	F	F
12.1140259837512527	2.5190489906166529	10.8353850732375427	F	F	F
10.5997628382328113	3.1291472501920117	11.7805097330318205	F	F	F
12.1140251451312189	0.6053776282217357	10.8353848893587461	F	F	F
12.1149432369080756	5.0915457164265909	14.7727853324124414	T	T	T
10.6004614497695293	2.5795491607576211	13.7211917973197792	T	T	T
12.1142858599247596	3.1228066770553471	14.8610839039826725	T	T	T
10.6008125969520037	0.6109427390916941	13.6738326928217493	T	T	T
10.6002544727252861	4.8827538692800614	17.5768489295050223	T	T	T
12.1150801995427724	2.5809956469529856	16.8175054792170258	T	T	T
10.5998461798011601	3.0642429342893398	17.9318628853461028	T	T	T
12.1142184355684304	0.6238145458604927	16.6800756649675002	T	T	T
15.1425434423237721	5.0428186788376976	8.9451241821253618	F	F	F
13.6282835202100525	2.5190490598409605	8.0000001838787966	F	F	F
15.1425439387676146	3.1291473194163189	8.9451248436730744	F	F	F
13.6282826815900187	0.6053776974460434	8.0000000000000000	F	F	F
13.6282859058649670	5.0428186096133896	11.7805090714841079	F	F	F
15.1425495478272527	2.5190489906166529	10.8353850732375427	F	F	F
13.6282864023088113	3.1291472501920117	11.7805097330318205	F	F	F
15.1425487092072171	0.6053776282217357	10.8353848893587461	F	F	F
15.1426648219831357	5.0920358265310455	14.7733814227023110	T	T	T
13.6285297207503273	2.5799054805791100	13.7217721706462701	T	T	T
15.1427619249207819	3.1232946510861148	14.8613206930056680	T	T	T
13.6289140476178918	0.6114333877095915	13.6739525727984361	T	T	T
13.6288066847051930	4.8851432566926745	17.5774008463274356	T	T	T
15.1429422833273684	2.5825556067244584	16.8178973724140981	T	T	T
13.6286333586403661	3.0667208584942109	17.9333356495614709	T	T	T
15.1428419334216802	0.6253311086608568	16.6803576215105096	T	T	T

```
Metal reference: ZnO(10-10)/fcc(100)_6x2/Cu E_tot= -130.39683582 eV
 D3-zero damping= -10.3044397 eV, D3-BJ damping= -13.0423422 eV
Cu
 1.0000000000000000
    15.1426178203800053    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.0475392734600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9359299014895974
  36
Cartesian
 -0.0000000395596081  0.0000000000000000  8.1843654721703682
  1.2620899597305120  1.2618848183650002  9.9726484737131145
  0.0000000000000000 -0.0000000000000000 11.7624268120926878
 -0.0000000634042485  2.5237696367300004  8.1843654721703682
  1.2620899597305111  3.7856544550950013  9.9726484737131145
  0.0000000185906646  2.5237696367300004 11.7624268120926878
  2.5234947040879740  0.0000000000000000  8.1842951264510422
  3.7856544550950013  1.2618848183650002  9.9724733003213490
  2.5237066522118039  0.0000000000000000 11.7624700471555474
  2.5234947040879740  2.5237696367300004  8.1842951264510422
  3.7856544550950013  3.7856544550950013  9.9724733003213490
  2.5237066760564448  2.5237696367300004 11.7624700101375144
  5.0478143038119008 -0.0000000000000000  8.1842950831590073
  6.3092189019134812  1.2618848183650002  9.9726488585128923
  5.0476022341335458 -0.0000000000000000 11.7624700745561164
  5.0478143038119008  2.5237696367300004  8.1842950963324004
  6.3092188870552413  3.7856544550950013  9.9726488585128923
  5.0476022341335458  2.5237696367300004 11.7624700526217616
  7.5713088675787663  0.0000000000000000  8.1843656292654980
  8.8333989580261516  1.2618848183650002  9.9726484984144861
  7.5713089497496133  0.0000000000000000 11.7624266783868432
  7.5713088706303919  2.5237696367300004  8.1843656054208545
  8.8333989580261516  3.7856544550950013  9.9726484984144861
  7.5713089497496133  2.5237696367300004 11.7624266783868432
 10.0948035747183837 -0.0000000000000000  8.1842951660106493
 11.3569633652850026  1.2618848183650002  9.9724733190879533
 10.0950155862464577 -0.0000000000000000 11.7624700249957481
 10.0948035747183837  2.5237696367300004  8.1842951336407186
 11.3569633652850026  3.7856544550950013  9.9724733190879533
 10.0950155862464577  2.5237696367300004 11.7624700261370947
 12.6191231984628569 -0.0000000000000000  8.1842950920184254
 13.8805278439945106  1.2618848183650002  9.9726488434292069
 12.6189110783777299  0.0000000000000000 11.7624700764664016
 12.6191231796962633  2.5237696367300004  8.1842950770483114
 13.8805278359481026  3.7856544550950013  9.9726488585128923
 12.6189110783777299  2.5237696367300004 11.7624700579011616

Interface: ZnO(10-10)/fcc(100)_6x2/Pt E_tot= -585.62164374 eV
 D3-zero damping= -35.9848324 eV, D3-BJ damping= -35.8141131 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Pt
 1.0000000000000000
    16.6227201925200028    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.5409067308400006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.3241942887299736
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2  36
Selective dynamics
Cartesian
  3.3244623904275628  5.5357247256887341  8.9451241821253618   F   F   F
  1.6621924128965724  2.7652713797353203  8.0000001838787966   F   F   F
  3.3244629353958910  3.4350031777085537  8.9451248436730744   F   F   F
  1.6621914923063332  0.6645498284909550  8.0000000000000000   F   F   F
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1.6621950317353087	5.5357246496981549	11.7805090714841079	F	F	F
3.3244690927083194	2.7652713037447412	10.8353850732375427	F	F	F
1.6621955767036365	3.4350031017179750	11.7805097330318205	F	F	F
3.3244681721180802	0.6645497525003760	10.8353848893587461	F	F	F
3.2968367902656084	5.4749222639622612	14.5070899924620491	T	T	T
1.6275736238627199	2.7396562697597648	13.6872759129536501	T	T	T
3.3245758276877342	3.4524155377929913	14.5437039661031715	T	T	T
1.6458872361250678	0.6948892128047741	13.6558046852827459	T	T	T
1.6130896592856536	5.6548457785137911	17.3655037233462970	T	T	T
3.3742296415984430	2.7248536861285064	16.4309552202097464	T	T	T
1.7931198966729101	3.6009157253830146	17.2923019816786478	T	T	T
3.2902745921744359	0.7325167801191215	16.3518154627417722	T	T	T
6.6490064289315631	5.5357247256887341	8.9451241821253618	F	F	F
4.9867364514005734	2.7652713797353203	8.0000001838787966	F	F	F
6.6490069738998914	3.4350031777085537	8.9451248436730744	F	F	F
4.9867355308103338	0.6645498284909550	8.0000000000000000	F	F	F
4.9867390702393095	5.5357246496981549	11.7805090714841079	F	F	F
6.6490131312123202	2.7652713037447412	10.8353850732375427	F	F	F
4.9867396152076378	3.4350031017179750	11.7805097330318205	F	F	F
6.6490122106220806	0.6645497525003760	10.8353848893587461	F	F	F
6.6378154343733247	5.4485188914483365	14.4725686270701086	T	T	T
4.9701816205305480	2.7089691255418940	13.6409708307224680	T	T	T
6.6495270965214406	3.4336147810577633	14.5037356341738466	T	T	T
4.9702484289203346	0.6752655006279662	13.6574123694274476	T	T	T
4.9404681524051055	5.5940211353705305	17.2107698498589308	T	T	T
6.6809301637842413	2.6833902193854282	16.3758441278416420	T	T	T
5.0715575689763650	3.5602542202933813	17.1664722772200875	T	T	T
6.6401681883468120	0.7010095564291955	16.3193483587732793	T	T	T
9.9735504674355635	5.5357247256887341	8.9451241821253618	F	F	F
8.3112804899045720	2.7652713797353203	8.0000001838787966	F	F	F
9.9735510124038917	3.4350031777085537	8.9451248436730744	F	F	F
8.3112795693143333	0.6645498284909550	8.0000000000000000	F	F	F
8.3112831087433108	5.5357246496981549	11.7805090714841079	F	F	F
9.9735571697163206	2.7652713037447412	10.8353850732375427	F	F	F
8.3112836537116372	3.4350031017179750	11.7805097330318205	F	F	F
9.9735562491260819	0.6645497525003760	10.8353848893587461	F	F	F
9.9837380185690616	5.4482743270081606	14.4727120176177930	T	T	T
8.3110124063338784	2.6978660483687307	13.6295359223313159	T	T	T
9.9724717696735503	3.4334392492984644	14.5038442086496708	T	T	T
8.3108787263369095	0.6688001001404608	13.6539353648656316	T	T	T
8.3110254289405070	5.5750918936630622	17.1849028586034045	T	T	T
9.9415347948287138	2.6833068885283100	16.3760736449169393	T	T	T
8.3111738394004391	3.5405844942393596	17.1580994604734585	T	T	T
9.9820048157977901	0.7008687700791030	16.3194695885564300	T	T	T
13.2980945059395648	5.5357247256887341	8.9451241821253618	F	F	F
11.6358245284085751	2.7652713797353203	8.0000001838787966	F	F	F
13.2980950509078948	3.4350031777085537	8.9451248436730744	F	F	F
11.6358236078183364	0.6645498284909550	8.0000000000000000	F	F	F
11.6358271472473120	5.5357246496981549	11.7805090714841079	F	F	F
13.2981012082203236	2.7652713037447412	10.8353850732375427	F	F	F
11.6358276922156403	3.4350031017179750	11.7805097330318205	F	F	F
13.2981002876300831	0.6645497525003760	10.8353848893587461	F	F	F
13.3252849775389119	5.4749189737561874	14.5070943064976063	T	T	T
11.6518414166433608	2.7087890427906895	13.6407872440121203	T	T	T
13.2976103171409132	3.4523686777022400	14.5433668228638364	T	T	T
11.6515991288614931	0.6750814522854581	13.6575658096561359	T	T	T
11.6819966511686122	5.5939259872118674	17.2109024343270285	T	T	T
13.2481007381999838	2.7248535152971129	16.4304287387122265	T	T	T
11.5509613449176349	3.5601534100094812	17.1665460182623058	T	T	T
13.3319809111115610	0.7324996124904618	16.3517472402011315	T	T	T
16.6226385444435678	5.5357247256887341	8.9451241821253618	F	F	F
14.9603685669125746	2.7652713797353203	8.0000001838787966	F	F	F
16.6226390894118943	3.4350031777085537	8.9451248436730744	F	F	F

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 14.9603676463223341  0.6645498284909550  8.0000000000000000   F   F   F
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 16.6226452467243213  2.7652713037447412 10.8353850732375427   F   F   F
 14.9603717307196380  3.4350031017179750 11.7805097330318205   F   F   F
 16.6226443261340826  0.6645497525003760 10.8353848893587461   F   F   F
 16.6223939854417644  5.4981138601164217 14.5478200610222679   T   T   T
 14.9946928846863372  2.7397714709871273 13.6871584221918621   T   T   T
 16.6225388630666266  3.4662619758205193 14.6784841464305327   T   T   T
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 15.0090017700480356  5.6548800188876855 17.3655962228753324   T   T   T
 16.6224910642614176  2.8052994854358451 16.6685626471881925   T   T   T
 14.8289878323426709  3.6009167000449280 17.2922195656612452   T   T   T
 16.6224169137893298  0.7917418296118129 16.3758579675823128   T   T   T
 -0.0004401171492401  0.6734288759555954 19.4877331946372436   T   T   T
  1.3787265203487029  2.0804714659929338 21.5099666133614527   T   T   T
 -0.0004192324056682  0.7123810192717139 23.5206231185273822   T   T   T
 -0.0003754324386015  3.4368691534359952 19.6485301555081371   T   T   T
  1.3866175867024151  4.8643343729051818 21.4985501033940096   T   T   T
 -0.0003986635060590  3.4937362830950560 23.4213120687418517   T   T   T
  2.7704789760465771  0.6692249372142567 19.5616380585809075   T   T   T
  4.1122951889721184  2.1930934237874897 21.3637768431511894   T   T   T
  2.7937538962893385  0.7478988221336570 23.3735814032682505   T   T   T
  2.6718979177148614  3.3655792375560281 19.2643366887604088   T   T   T
  4.1493863780918110  4.8614428733056467 21.4116042333810448   T   T   T
  2.8046215168549877  3.5123704747269651 23.4301545404684006   T   T   T
  5.5503346732174350  0.7003144540795270 19.5393374129214337   T   T   T
  6.9007087589272649  2.2336420424703949 21.3508127176969147   T   T   T
  5.5369396684479568  0.8194515880023855 23.3080134148261351   T   T   T
  5.4598174017382544  3.3898428761960138 19.2211798729953784   T   T   T
  6.9227070082196320  4.8974262572543550 21.4092111459909198   T   T   T
  5.5386490169306564  3.5547999019016121 23.3628969408490761   T   T   T
  8.3107824680016176  0.7433133468522487 19.5623133080981084   T   T   T
  9.7212315757723999  2.2336363147473630 21.3505181632915999   T   T   T
  8.3107365737070698  0.8511251583318038 23.3028446847785489   T   T   T
  8.3109627020562620  3.4406885528724631 19.2502261180710690   T   T   T
  9.6989503001701838  4.8976686707416910 21.4091179411955324   T   T   T
  8.3108591122160735  3.5794303405017938 23.3552150430762175   T   T   T
 11.0711685303592891  0.7002247925491485 19.5392847201795519   T   T   T
 12.5094328818239546  2.1931796349245598 21.3640623685558708   T   T   T
 11.0845980456037818  0.8199335397483274 23.3082980310164380   T   T   T
 11.1625369389143376  3.3896684364781011 19.2212726319661833   T   T   T
 12.4725057003394770  4.8618743102254962 21.4121665754908719   T   T   T
 11.0827796548348765  3.5551254755599766 23.3630060883597395   T   T   T
 13.8513004427382391  0.6689671804354465 19.5618453205595522   T   T   T
 15.2430002051013123  2.0809614827107996 21.5098907467573497   T   T   T
 13.8280267855249566  0.7486127010557492 23.3736937687873692   T   T   T
 13.9500018143339890  3.3655363706781358 19.2644253572296300   T   T   T
 15.2357032917374156  4.8648254383906817 21.4987146574987591   T   T   T
 13.8173809151906433  3.5133512301142833 23.4303916447292906   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_6x2/Pt E_tot= -357.78165056 eV
 D3-zero damping= -12.7264046 eV, D3-BJ damping= -13.638142 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
    16.6227201925200028    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.5409067308400006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.1312880290811052
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2
Selective dynamics
Cartesian
```

3.3244623904275628	5.5357247256887341	8.9451241821253618	F	F	F
1.6621924128965724	2.7652713797353203	8.0000001838787966	F	F	F
3.3244629353958910	3.4350031777085537	8.9451248436730744	F	F	F
1.6621914923063332	0.6645498284909550	8.0000000000000000	F	F	F
1.6621950317353087	5.5357246496981549	11.7805090714841079	F	F	F
3.3244690927083194	2.7652713037447412	10.8353850732375427	F	F	F
1.6621955767036365	3.4350031017179750	11.7805097330318205	F	F	F
3.3244681721180802	0.6645497525003760	10.8353848893587461	F	F	F
3.3239299312931374	5.4394414513073661	14.4686620887813149	T	T	T
1.6619332878473054	2.7275789463746398	13.6708270281269471	T	T	T
3.3240852254115576	3.4267283150663319	14.5378577627024015	T	T	T
1.6626772977841786	0.6742641826925511	13.6674361490872496	T	T	T
1.6613130709221862	5.2354020482432952	16.9196500131889316	T	T	T
3.3255471297429193	2.6622861811587324	16.5193317937763098	T	T	T
1.6631138543311248	3.3820033837928047	17.2313456008318262	T	T	T
3.3232444469659055	0.6228599116743900	16.4282932319299348	T	T	T
6.6490064289315631	5.5357247256887341	8.9451241821253618	F	F	F
4.9867364514005734	2.7652713797353203	8.0000001838787966	F	F	F
6.6490069738998914	3.4350031777085537	8.9451248436730744	F	F	F
4.9867355308103338	0.6645498284909550	8.0000000000000000	F	F	F
4.9867390702393095	5.5357246496981549	11.7805090714841079	F	F	F
6.6490131312123202	2.7652713037447412	10.8353850732375427	F	F	F
4.9867396152076378	3.4350031017179750	11.7805097330318205	F	F	F
6.6490122106220806	0.6645497525003760	10.8353848893587461	F	F	F
6.6501280286597888	5.4384014590021676	14.4689933669140878	T	T	T
4.9864527571970161	2.7276220498095856	13.6707493884863567	T	T	T
6.6488470886461526	3.4262316606110650	14.5382918637609730	T	T	T
4.9874742793800015	0.6740196428706970	13.6675717700466617	T	T	T
4.9862445625101017	5.2359758308862876	16.9206948445726510	T	T	T
6.6503820381835315	2.6632714744412262	16.5192886716426734	T	T	T
4.9878254517357075	3.3826038944870493	17.2311571686842271	T	T	T
6.6481941683252543	0.6232661067489672	16.4278833118610699	T	T	T
9.9735504674355635	5.5357247256887341	8.9451241821253618	F	F	F
8.3112804899045720	2.7652713797353203	8.0000001838787966	F	F	F
9.9735510124038917	3.4350031777085537	8.9451248436730744	F	F	F
8.3112795693143333	0.6645498284909550	8.0000000000000000	F	F	F
8.3112831087433108	5.5357246496981549	11.7805090714841079	F	F	F
9.9735571697163206	2.7652713037447412	10.8353850732375427	F	F	F
8.3112836537116372	3.4350031017179750	11.7805097330318205	F	F	F
9.9735562491260819	0.6645497525003760	10.8353848893587461	F	F	F
9.9724736282237636	5.4384198519935936	14.4690279392959837	T	T	T
8.3113222948782361	2.7277133944376728	13.6702114067407763	T	T	T
9.9737385658144913	3.4262304503461847	14.5383264897811397	T	T	T
8.3113115020253741	0.6742626166238139	13.6673015867655536	T	T	T
8.3112895326510330	5.2381375862292527	16.9209856218240091	T	T	T
9.9722412259323345	2.6631698654598672	16.5192877763294526	T	T	T
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9.9744093705348202	0.6232930003903806	16.4279253987716878	T	T	T
13.2980945059395648	5.5357247256887341	8.9451241821253618	F	F	F
11.6358245284085751	2.7652713797353203	8.0000001838787966	F	F	F
13.2980950509078948	3.4350031777085537	8.9451248436730744	F	F	F
11.6358236078183364	0.6645498284909550	8.0000000000000000	F	F	F
11.6358271472473120	5.5357246496981549	11.7805090714841079	F	F	F
13.2981012082203236	2.7652713037447412	10.8353850732375427	F	F	F
11.6358276922156403	3.4350031017179750	11.7805097330318205	F	F	F
13.2981002876300831	0.6645497525003760	10.8353848893587461	F	F	F
13.2986227928642595	5.4394243010531724	14.4686709664217759	T	T	T
11.6361094021065998	2.7276190466437416	13.6707466151945862	T	T	T
13.2984941088986677	3.4266952420102443	14.5378777123640646	T	T	T
11.6351300962070674	0.6740113409788721	13.6675991637382772	T	T	T
11.6363376259103450	5.2360418218180715	16.9207777968554076	T	T	T
13.2970612053045709	2.6622743456777354	16.5193821865698212	T	T	T
11.6348148742618154	3.3825788222893682	17.2311433107556269	T	T	T

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 13.2992974935052004  0.6228321297662955 16.4282705991009834   T   T   T
 16.6226385444435678  5.5357247256887341  8.9451241821253618   F   F   F
 14.9603685669125746  2.7652713797353203  8.0000001838787966   F   F   F
 16.6226390894118943  3.4350031777085537  8.9451248436730744   F   F   F
 14.9603676463223341  0.6645498284909550  8.0000000000000000   F   F   F
 14.9603711857513115  5.5357246496981549 11.7805090714841079   F   F   F
 16.6226452467243213  2.7652713037447412 10.8353850732375427   F   F   F
 14.9603717307196380  3.4350031017179750 11.7805097330318205   F   F   F
 16.6226443261340826  0.6645497525003760 10.8353848893587461   F   F   F
 16.6226747767700402  5.4383935597840063 14.4692326627148375   T   T   T
 14.9606156147727773  2.7276086263748267 13.6708243400305847   T   T   T
 16.6226455985605952  3.4266022303185064 14.5387112109685752   T   T   T
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 14.9612764427740217  5.2354175921092576 16.9196063338847758   T   T   T
 16.6226772623173034  2.6624533343134393 16.5207183871341954   T   T   T
 14.9594644580507499  3.3820412991604543 17.2313293612529499   T   T   T
 16.6226529738968587  0.6228035982064669 16.4281986854464428   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_6x2/Pt E_tot= -215.19930717 eV
 D3-zero damping= -16.5053143 eV, D3-BJ damping= -17.2965978 eV
Pt
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    16.6227201925200028    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.5409067308400006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9359299014895974
  36
Cartesian
  0.0000000323553548  0.0000000000000000  8.0284670942930720
  1.3852266593107860  1.3852266827100002  9.9731569497610177
  0.0000000619642757  0.0000000000000000 11.9177404277913546
  0.0000000213735893  2.7704533654200003  8.0284670110103331
  1.3852266593107860  4.1556800481300007  9.9731569497610177
  0.0000001282833435  2.7704533654200003 11.9177403445086156
  2.7704533674475922  0.0000000000000000  8.0284670229416086
  4.1556799308284207  1.3852266557120974  9.9731569161341724
  2.7704533519597496  0.0000000000000000 11.9177404030105070
  2.7704534337666615  2.7704533654200003  8.0284671052768122
  4.1556799317759472  4.1556800751278979  9.9731569161341724
  2.7704533519597496  2.7704533654200003 11.9177403428049900
  5.5409067316922576 -0.0000000000000000  8.0284670383743126
  6.9261334120741820  1.3852266871199230  9.9731569025413922
  5.5409067477083944  0.0000000000000000 11.9177403879017465
  5.5409067586901548  2.7704533654200003  8.0284670714857764
  6.9261333798140985  4.1556800437200723  9.9731569025413922
  5.5409067316922576  2.7704533654200003 11.9177404039178825
  8.3113600206628018 -0.0000000000000000  8.0284670555657947
  9.6965867294222914  1.3852266871199230  9.9731569188806084
  8.3113600800160583 -0.0000000000000000 11.9177404233964204
  8.3113600206628018  2.7704533654200003  8.0284671020422191
  9.6965866819983297  4.1556800437200723  9.9731569188806084
  8.3113600962600014  2.7704533654200003 11.9177404664104554
 11.0818133962123078 -0.0000000000000000  8.0284669817655310
 12.4670401425910935  1.3852266827100002  9.9731569388194021
 11.0818133971598325 -0.0000000000000000 11.9177405793021087
 11.0818134134037845  2.7704533654200003  8.0284670140256118
 12.4670401748511797  4.1556800481300007  9.9731569388194021
 11.0818133497358708  2.7704533654200003 11.9177405460944961
 13.8522667851267887  0.0000000000000000  8.0284669772193080
 15.2374936342668388  1.3852266827100002  9.9731569703233802
 13.8522668396127209  0.0000000000000000 11.9177405065829980
 13.8522668011429264  2.7704533654200003  8.0284669772193080
 15.2374936342668388  4.1556800481300007  9.9731569433254794
 13.8522668396127209  2.7704533654200003 11.9177405810048604
```

```
Interface: ZnO(10-10)/fcc(100)_6x2/Pd E_tot= -552.87755162 eV
 D3-zero damping= -31.379971 eV, D3-BJ damping= -33.4741002 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Pd
 1.0000000000000000
    16.4878873914000046    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4959624638000006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.3241942887299736
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2  36
Selective dynamics
Cartesian
  3.2974964924801777  5.4908224917372941  8.9451241821253618   F   F   F
  1.6487097785000613  2.7428412791459800  8.0000001838787966   F   F   F
  3.2974970330280740  3.4071406440833432  8.9451248436730744   F   F   F
  1.6487088653770572  0.6591594282543216  8.0000000000000000   F   F   F
  1.6487123760964641  5.4908224163631019 11.7805090714841079   F   F   F
  3.2975031403963495  2.7428412037717878 10.8353850732375427   F   F   F
  1.6487129166443599  3.4071405687091514 11.7805097330318205   F   F   F
  3.2975022272733452  0.6591593528801291 10.8353848893587461   F   F   F
  3.2781690387642599  5.4175122577814472 14.5262662114882311   T   T   T
  1.6338174700318968  2.7085175242028567 13.6737562488596414   T   T   T
  3.2943546946461235  3.4072294828297034 14.5745348887025568   T   T   T
  1.6410080789270896  0.6776427186789178 13.6599582263762152   T   T   T
  1.6012124835092529  5.5517066966588668 17.3584956643250479   T   T   T
  3.3029806987700705  2.6989956591650976 16.4861593249694423   T   T   T
  1.6931595708611054  3.5486246913809381 17.3004740897997635   T   T   T
  3.2616562199340891  0.7067059898397811 16.3846900476577950   T   T   T
  6.5950739707601782  5.4908224917372941  8.9451241821253618   F   F   F
  4.9462872567800629  2.7428412791459800  8.0000001838787966   F   F   F
  6.5950745113080753  3.4071406440833432  8.9451248436730744   F   F   F
  4.9462863436570590  0.6591594282543216  8.0000000000000000   F   F   F
  4.9462898543764657  5.4908224163631019 11.7805090714841079   F   F   F
  6.5950806186763504  2.7428412037717878 10.8353850732375427   F   F   F
  4.9462903949243620  3.4071405687091514 11.7805097330318205   F   F   F
  6.5950797055533457  0.6591593528801291 10.8353848893587461   F   F   F
  6.5852603243800436  5.3883289103155176 14.5069177336003783   T   T   T
  4.9332697094856011  2.6867793264212212 13.6550577865111187   T   T   T
  6.5939710817915689  3.3817700399132731 14.5461969049076973   T   T   T
  4.9355250759105589  0.6578332054234504 13.6658407326260729   T   T   T
  4.8839580731169132  5.4718850148348555 17.2445672271636781   T   T   T
  6.6034424029796286  2.6393944017335818 16.4424979670924074   T   T   T
  4.9876149270235395  3.4819081580192504 17.2120936385344798   T   T   T
  6.5764020953218854  0.6558328304387020 16.3758132290050185   T   T   T
  9.8926514490401800  5.4908224917372941  8.9451241821253618   F   F   F
  8.2438647350600629  2.7428412791459800  8.0000001838787966   F   F   F
  9.8926519895880762  3.4071406440833432  8.9451248436730744   F   F   F
  8.2438638219370581  0.6591594282543216  8.0000000000000000   F   F   F
  8.2438673326564675  5.4908224163631019 11.7805090714841079   F   F   F
  9.8926580969563513  2.7428412037717878 10.8353850732375427   F   F   F
  8.2438678732043620  3.4071405687091514 11.7805097330318205   F   F   F
  9.8926571838333466  0.6591593528801291 10.8353848893587461   F   F   F
  9.9024480490723779  5.3883776685093325 14.5069244480238826   T   T   T
  8.2438124364172953  2.6772176815128299 13.6466555067104860   T   T   T
  9.8937938439066517  3.3816944087810494 14.5461511211302845   T   T   T
  8.2438444656803949  0.6481743140030840 13.6676697965768650   T   T   T
  8.2439009497111098  5.4522095848974255 17.2047091752742531   T   T   T
  9.8843752478099329  2.6392763204194467 16.4423968434221202   T   T   T
  8.2439747185944245  3.4577504413707585 17.1862240411847225   T   T   T
  9.9114110671002482  0.6557448859273121 16.3757400727445663   T   T   T
 13.1902289273201809  5.4908224917372941  8.9451241821253618   F   F   F
```

11.5414422133400656	2.7428412791459800	8.0000001838787966	F	F	F
13.1902294678680789	3.4071406440833432	8.9451248436730744	F	F	F
11.5414413002170608	0.6591594282543216	8.0000000000000000	F	F	F
11.5414448109364685	5.4908224163631019	11.7805090714841079	F	F	F
13.1902355752363540	2.7428412037717878	10.8353850732375427	F	F	F
11.5414453514843647	3.4071405687091514	11.7805097330318205	F	F	F
13.1902346621133510	0.6591593528801291	10.8353848893587461	F	F	F
13.2095747297138999	5.4173355818461770	14.5262512636985335	T	T	T
11.5544922442655729	2.6867093835697404	13.6550060216990214	T	T	T
13.1934243196137508	3.4070757988798288	14.5745426021827367	T	T	T
11.5522096493449542	0.6577494236523496	13.6658531695808723	T	T	T
11.6037935644036203	5.4717174695485928	17.2444338312609560	T	T	T
13.1848335644771044	2.6987549910812385	16.4861793177208895	T	T	T
11.5002160251224712	3.4817463152499175	17.2119807831371894	T	T	T
13.2261969596127500	0.7064933460001405	16.3846530801887624	T	T	T
16.4878064056001854	5.4908224917372941	8.9451241821253618	F	F	F
14.8390196916200647	2.7428412791459800	8.0000001838787966	F	F	F
16.4878069461480798	3.4071406440833432	8.9451248436730744	F	F	F
14.8390187784970617	0.6591594282543216	8.0000000000000000	F	F	F
14.8390222892164694	5.4908224163631019	11.7805090714841079	F	F	F
16.4878130535163550	2.7428412037717878	10.8353850732375427	F	F	F
14.8390228297643638	3.4071405687091514	11.7805097330318205	F	F	F
16.4878121403933484	0.6591593528801291	10.8353848893587461	F	F	F
16.4878797785321431	5.4394912416411438	14.5408111617998070	T	T	T
14.8539681219372408	2.7084668469309401	13.6736834026116441	T	T	T
16.4878397357864266	3.4260978504208550	14.6207520798428341	T	T	T
14.8467417658716965	0.6775799074967834	13.6599958718989427	T	T	T
14.8867190232219961	5.5516305214036130	17.3583471177601254	T	T	T
16.4878041206592947	2.7592331218697748	16.5632288159689232	T	T	T
14.7945930599601567	3.5484989467277819	17.3004520053343605	T	T	T
16.4879194237091902	0.7557720929481382	16.3852535828249977	T	T	T
0.0001475560449209	0.9311965871573009	19.3813184430647887	T	T	T
1.3728606218002755	2.2986509774860306	21.3696948321480242	T	T	T
0.0001216140782779	0.9254245732347036	23.3555899939504528	T	T	T
0.0001178921500368	3.6702032079907774	19.4443281354811646	T	T	T
1.3742159922319797	5.0552372733755826	21.3620423316636092	T	T	T
0.0000979303409215	3.6758422142823348	23.3040712046521179	T	T	T
2.7812545472979728	0.9588064493023768	19.4365247023777741	T	T	T
4.1143803744033605	2.3338221469967868	21.3612358310719159	T	T	T
2.7410146654686391	0.9259217550264116	23.3049544058807143	T	T	T
2.7255204786546221	3.6778971134253378	19.3075090398396405	T	T	T
4.1143253367339270	5.0309789266050364	21.3332203668840954	T	T	T
2.7485437841306641	3.6817790773899177	23.3282902859311818	T	T	T
5.5310778804933003	0.9697187269806186	19.4585893408536528	T	T	T
6.8650070768914837	2.3375611515489232	21.3847820544424145	T	T	T
5.4809227917040833	0.9197337634520660	23.2911888918187380	T	T	T
5.4879629591722088	3.6746141841046049	19.2856687723829516	T	T	T
6.8643585615882303	5.0156118411627721	21.3348516817682246	T	T	T
5.4887981563281558	3.6851578615827503	23.3321845797806553	T	T	T
8.2439834536165542	0.9694524374372288	19.4870173726960516	T	T	T
9.6231648161436141	2.3375800478673514	21.3847160307804778	T	T	T
8.2440693910842917	0.9133040852770432	23.2892963177724326	T	T	T
8.2440062089968897	3.6635475508837652	19.2861559822196220	T	T	T
9.6237629705055117	5.0156442787816546	21.3346618885784949	T	T	T
8.2441870809988043	3.6828417949732231	23.3377580827683353	T	T	T
10.9571901508237612	0.9696194003530698	19.4584878432117030	T	T	T
12.3738169867271921	2.3338363141886673	21.3611484849423121	T	T	T
11.0071562526306526	0.9195424552342593	23.2909901016984122	T	T	T
11.0001082091661004	3.6744890117127769	19.2855590403600452	T	T	T
12.3738198475747030	5.0307790175520521	21.3331419724845581	T	T	T
10.9993878198337569	3.6851407373528375	23.3321036227261800	T	T	T
13.7069235631779911	0.9587032642832143	19.4366280257856836	T	T	T
15.1154204138086161	2.2985808791818725	21.3696483815555673	T	T	T

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 13.7470648928130164  0.9257366203346830 23.3048329870083393   T   T   T
 13.7625795770639172  3.6776475834006952 19.3074718011576074   T   T   T
 15.1138884206889887  5.0553208588010987 21.3620853754826996   T   T   T
 13.7396564624841702  3.6816327610299227 23.3284081167711719   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_6x2/Pd E_tot= -358.47282481 eV
 D3-zero damping= -12.8037869 eV, D3-BJ damping= -13.8129276 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
    16.4878873914000046    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4959624638000006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.1312880290811052
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2
Selective dynamics
Cartesian
  3.2974964924801777  5.4908224917372941  8.9451241821253618   F   F   F
  1.6487097785000613  2.7428412791459800  8.0000001838787966   F   F   F
  3.2974970330280740  3.4071406440833432  8.9451248436730744   F   F   F
  1.6487088653770572  0.6591594282543216  8.0000000000000000   F   F   F
  1.6487123760964641  5.4908224163631019 11.7805090714841079   F   F   F
  3.2975031403963495  2.7428412037717878 10.8353850732375427   F   F   F
  1.6487129166443599  3.4071405687091514 11.7805097330318205   F   F   F
  3.2975022272733452  0.6591593528801291 10.8353848893587461   F   F   F
  3.2973166716989715  5.4034408776841403 14.4942224528830188   T   T   T
  1.6473153080749747  2.7096971769346418 13.6743251950223250   T   T   T
  3.2958832396538771  3.3984726418168645 14.5654998050750510   T   T   T
  1.6492461904793154  0.6697338683293613 13.6676482052432888   T   T   T
  1.6468216491332914  5.1958156703194298 16.9722856354764744   T   T   T
  3.2971955203891037  2.6467037480996312 16.5449901190529403   T   T   T
  1.6487262109421068  3.3498132849014222 17.2924000677251080   T   T   T
  3.2961503538090886  0.6197281620412313 16.4490596937955864   T   T   T
  6.5950739707601782  5.4908224917372941  8.9451241821253618   F   F   F
  4.9462872567800629  2.7428412791459800  8.0000001838787966   F   F   F
  6.5950745113080753  3.4071406440833432  8.9451248436730744   F   F   F
  4.9462863436570590  0.6591594282543216  8.0000000000000000   F   F   F
  4.9462898543764657  5.4908224163631019 11.7805090714841079   F   F   F
  6.5950806186763504  2.7428412037717878 10.8353850732375427   F   F   F
  4.9462903949243620  3.4071405687091514 11.7805097330318205   F   F   F
  6.5950797055533457  0.6591593528801291 10.8353848893587461   F   F   F
  6.5960430189968768  5.4036109511016486 14.4950913934791590   T   T   T
  4.9450221912381656  2.7102427716702673 13.6744743045129677   T   T   T
  6.5947531574536473  3.3983425163372840 14.5642036826028516   T   T   T
  4.9466560504885182  0.6693820057059103 13.6683793185333649   T   T   T
  4.9455460530591671  5.1970391432323648 16.9724598868688048   T   T   T
  6.5967616087705814  2.6471158972570694 16.5431726916675963   T   T   T
  4.9473980130515027  3.3502832129123559 17.2897905509190295   T   T   T
  6.5947127476167982  0.6200656458123422 16.4495835603289393   T   T   T
  9.8926514490401800  5.4908224917372941  8.9451241821253618   F   F   F
  8.2438647350600629  2.7428412791459800  8.0000001838787966   F   F   F
  9.8926519895880762  3.4071406440833432  8.9451248436730744   F   F   F
  8.2438638219370581  0.6591594282543216  8.0000000000000000   F   F   F
  8.2438673326564675  5.4908224163631019 11.7805090714841079   F   F   F
  9.8926580969563513  2.7428412037717878 10.8353850732375427   F   F   F
  8.2438678732043620  3.4071405687091514 11.7805097330318205   F   F   F
  9.8926571838333466  0.6591593528801291 10.8353848893587461   F   F   F
  9.8915847187168904  5.4036778176348204 14.4951126537505921   T   T   T
  8.2437517081023213  2.7088482190328818 13.6729922009392730   T   T   T
  9.8928216440597190  3.3983007386678672 14.5641790390507353   T   T   T
  8.2437636939421139  0.6692264121738617 13.6679944783058946   T   T   T
  8.2435810149816842  5.1968639274955022 16.9757193619590794   T   T   T
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  9.8906013137070357  2.6470750445800291 16.5432317862780316   T   T   T
  8.2436982393585687  3.3506550814605438 17.2929044139657009   T   T   T
  9.8926083669503200  0.6199869555801901 16.4496005217584980   T   T   T
 13.1902289273201809  5.4908224917372941  8.9451241821253618   F   F   F
 11.5414422133400656  2.7428412791459800  8.0000001838787966   F   F   F
 13.1902294678680789  3.4071406440833432  8.9451248436730744   F   F   F
 11.5414413002170608  0.6591594282543216  8.0000000000000000   F   F   F
 11.5414448109364685  5.4908224163631019 11.7805090714841079   F   F   F
 13.1902355752363540  2.7428412037717878 10.8353850732375427   F   F   F
 11.5414453514843647  3.4071405687091514 11.7805097330318205   F   F   F
 13.1902346621133510  0.6591593528801291 10.8353848893587461   F   F   F
 13.1901393026705129  5.4034398516491171 14.4941876975154660   T   T   T
 11.5425823575112201  2.7102346536599797 13.6744411604193150   T   T   T
 13.1916969361928995  3.3984728395021007 14.5654581515328303   T   T   T
 11.5408552276196925  0.6693840306173610 13.6683546528113560   T   T   T
 11.5417936083426920  5.1969902059060678 16.9724222578764525   T   T   T
 13.1902391385674971  2.6465701180203398 16.5448991949986777   T   T   T
 11.5401044772658139  3.3502220531563802 17.2897005201100740   T   T   T
 13.1912552893652180  0.6196400176360043 16.4490261313456152   T   T   T
 16.4878064056001854  5.4908224917372941  8.9451241821253618   F   F   F
 14.8390196916200647  2.7428412791459800  8.0000001838787966   F   F   F
 16.4878069461480798  3.4071406440833432  8.9451248436730744   F   F   F
 14.8390187784970617  0.6591594282543216  8.0000000000000000   F   F   F
 14.8390222892164694  5.4908224163631019 11.7805090714841079   F   F   F
 16.4878130535163550  2.7428412037717878 10.8353850732375427   F   F   F
 14.8390228297643638  3.4071405687091514 11.7805097330318205   F   F   F
 16.4878121403933484  0.6591593528801291 10.8353848893587461   F   F   F
 16.4876659813500197  5.4047416821506298 14.4922974292365687   T   T   T
 14.8402099564981231  2.7096844575382297 13.6742315121266849   T   T   T
 16.4876989344118812  3.3999589083992281 14.5656226372405264   T   T   T
 14.8382447349720508  0.6697398068958424 13.6676308924374403   T   T   T
 14.8407835215582793  5.1957940923608774 16.9722104991256728   T   T   T
 16.4875799585544662  2.6465701485608815 16.5452962604227309   T   T   T
 14.8386794114286502  3.3497474912821583 17.2924567487174734   T   T   T
 16.4876474820449630  0.6204641060388956 16.4478217562750153   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_6x2/Pd E_tot= -182.74222942 eV
 D3-zero damping= -12.2294196 eV, D3-BJ damping= -14.9413193 eV
Pd
 1.0000000000000000
    16.4878873914000046    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4959624638000006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9359299014895974
  36
Cartesian
  0.0000000000000000 -0.0000000333558865  8.0180052093007230
  1.3739907609443216  1.3739906159500002  9.9734134207475975
  0.0000000183697332 -0.0000000333558865 11.9279456146577747
  0.0000000000000000  2.7479812652558868  8.0180052426566011
  1.3739906962118744  4.1219718478500011  9.9734134207475975
  0.0000000000000000  2.7479812652558868 11.9279456448349137
  2.7479811671675511 -0.0000000333558865  8.0180053542950311
  4.1219718478500011  1.3739906159500002  9.9734136109052276
  2.7479812502697305 -0.0000000333558865 11.9279455829427654
  2.7479811671675511  2.7479812652558868  8.0180052878198946
  4.1219718144941151  4.1219718478500011  9.9734136109052276
  2.7479812502697305  2.7479812652558868 11.9279456660449537
  5.4959623669110886 -0.0000000000000000  8.0180051839432096
  6.8699530026668763  1.3739906159500002  9.9734137029744954
  5.4959624002669747  0.0000000000000000 11.9279457020045037
  5.4959623219844262  2.7479812319000003  8.0180052924029113
  6.8699530613802677  4.1219718478500011  9.9734137225436577
  5.4959623669110886  2.7479812319000003 11.9279456189023367
```

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  8.2439437604324493 -0.0000000000000000  8.0180052936023252
  9.6179343116500018  1.3739906159500002  9.9734135461727806
  8.2439436125978229 -0.0000000000000000 11.9279457020045037
  8.2439437290558786  2.7479812319000003  8.0180053122086843
  9.6179343116500018  4.1219718478500011  9.9734135461727806
  8.2439436773302699  2.7479812319000003 11.9279455843470199
 10.9919250440580658 -0.0000000000000000  8.0180053269582103
 12.3659154650308150  1.3739906159500002  9.9734134207475975
 10.9919249609558776  0.0000000000000000 11.9279454860538454
 10.9919249609558776  2.7479812319000003  8.0180052438560221
 12.3659155285638498  4.1219718478500011  9.9734134207475975
 10.9919249609558776  2.7479812319000003 11.9279456474385768
 13.7399062230330298 -0.0000000000000000  8.0180052378369648
 15.1138968056271512  1.3739906159500002  9.9734134854800445
 13.7399062829458423  0.0000000000000000 11.9279457095673624
 13.7399061896771535  2.7479812319000003  8.0180052562067061
 15.1138968389830275  4.1219718478500011  9.9734134854800445
 13.7399062829458423  2.7479812652558868 11.9279456450715511

Interface: ZnO(10-10)/fcc(100)_6x2/Ir E_tot= -674.3374809 eV
 D3-zero damping= -34.2731334 eV, D3-BJ damping= -35.1382965 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Ir
 1.0000000000000000
    16.2903792873000057    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4301264291000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.3241942887299736
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2  36
Selective dynamics
Cartesian
  3.2579958417876056  5.4250480286694351  8.9451241821253618   F   F   F
  1.6289599139581354  2.7099848331968222  8.0000001838787966   F   F   F
  3.2579963758602881  3.3663265680868064  8.9451248436730744   F   F   F
  1.6289590117734154  0.6512633694152701  8.0000000000000000   F   F   F
  1.6289624804379781  5.4250479541981491 11.7805090714841079   F   F   F
  3.2580024100685101  2.7099847587255361 10.8353850732375427   F   F   F
  1.6289630145106604  3.3663264936155204 11.7805097330318205   F   F   F
  3.2580015078837898  0.6512632949439837 10.8353848893587461   F   F   F
  3.2346273521821352  5.3918349351177994 14.5530959938591291   T   T   T
  1.6014148136955824  2.7035211280531333 13.7082176885209250   T   T   T
  3.2616360718680699  3.3872189873715959 14.6273377108573754   T   T   T
  1.6129334781459834  0.6863981160070858 13.6525374380256324   T   T   T
  1.5818445494846780  5.6236979322293514 17.4525029890830261   T   T   T
  3.3185849448598477  2.7152015453231928 16.5340539199393177   T   T   T
  1.7746794631428020  3.5632486588687926 17.4837701709824813   T   T   T
  3.2238289323163132  0.7360193635070806 16.3878132023655851   T   T   T
  6.5160716992476067  5.4250480286694351  8.9451241821253618   F   F   F
  4.8870357714181374  2.7099848331968222  8.0000001838787966   F   F   F
  6.5160722333202896  3.3663265680868064  8.9451248436730744   F   F   F
  4.8870348692334167  0.6512633694152701  8.0000000000000000   F   F   F
  4.8870383378979794  5.4250479541981491 11.7805090714841079   F   F   F
  6.5160782675285107  2.7099847587255361 10.8353850732375427   F   F   F
  4.8870388719706632  3.3663264936155204 11.7805097330318205   F   F   F
  6.5160773653437909  0.6512632949439837 10.8353848893587461   F   F   F
  6.5050525308936900  5.3538360677211561 14.5174382000398392   T   T   T
  4.8748322266671744  2.6736520659847902 13.6624548592493262   T   T   T
  6.5191547622210564  3.3555999724522438 14.5891121483103081   T   T   T
  4.8709072112977143  0.6638054241622837 13.6519241699841665   T   T   T
  4.8361833605603657  5.5057634964288313 17.3238480128298349   T   T   T
  6.5459527258927661  2.6369831101460708 16.4740161295063707   T   T   T
  4.9975021627237393  3.4795035998851134 17.3681341185659619   T   T   T
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6.5013810646724233	0.6715945158467179	16.3562506063490538	T	T	T
9.7741475567076090	5.4250480286694351	8.9451241821253618	F	F	F
8.1451116288781371	2.7099848331968222	8.0000001838787966	F	F	F
9.7741480907802902	3.3663265680868064	8.9451248436730744	F	F	F
8.1451107266934173	0.6512633694152701	8.0000000000000000	F	F	F
8.1451141953579818	5.4250479541981491	11.7805090714841079	F	F	F
9.7741541249885131	2.7099847587255361	10.8353850732375427	F	F	F
8.1451147294306629	3.3663264936155204	11.7805097330318205	F	F	F
9.7741532228037933	0.6512632949439837	10.8353848893587461	F	F	F
9.7852660392381345	5.3538149021353156	14.5173975778696764	T	T	T
8.1451488605172280	2.6591846723379260	13.6498269336945324	T	T	T
9.7712726050790231	3.3554966222178724	14.5890834076947833	T	T	T
8.1451565692608856	0.6526212510929725	13.6499966141509894	T	T	T
8.1449901594526235	5.4673267593420656	17.2788455867770168	T	T	T
9.7445440167060138	2.6368965782473572	16.4739406514155107	T	T	T
8.1452439575711892	3.4419274463898040	17.3500362422772270	T	T	T
9.7886694287996843	0.6714789538480481	16.3563053244943220	T	T	T
13.0322234141676105	5.4250480286694351	8.9451241821253618	F	F	F
11.4031874863381404	2.7099848331968222	8.0000001838787966	F	F	F
13.0322239482402935	3.3663265680868064	8.9451248436730744	F	F	F
11.4031865841534206	0.6512633694152701	8.0000000000000000	F	F	F
11.4031900528179833	5.4250479541981491	11.7805090714841079	F	F	F
13.0322299824485164	2.7099847587255361	10.8353850732375427	F	F	F
11.4031905868906662	3.3663264936155204	11.7805097330318205	F	F	F
13.0322290802637966	0.6512632949439837	10.8353848893587461	F	F	F
13.0557214175190222	5.3916474224219257	14.5530729275206543	T	T	T
11.4156458029458694	2.6734448528380179	13.6624662473986920	T	T	T
13.0287552411220791	3.3871011628959486	14.6272911035136470	T	T	T
11.4194647657525543	0.6636481682374117	13.6519779715568497	T	T	T
11.4540515225814907	5.5057610104897057	17.3237301921543398	T	T	T
12.9717755499709355	2.7151167306792798	16.5339311916406082	T	T	T
11.2930009215110427	3.4794141730757082	17.3681259794357459	T	T	T
13.0662216819095232	0.7360148053488486	16.3876763035591750	T	T	T
16.2902992716276138	5.4250480286694351	8.9451241821253618	F	F	F
14.6612633437981401	2.7099848331968222	8.0000001838787966	F	F	F
16.2902998057002932	3.3663265680868064	8.9451248436730744	F	F	F
14.6612624416134203	0.6512633694152701	8.0000000000000000	F	F	F
14.6612659102779848	5.4250479541981491	11.7805090714841079	F	F	F
16.2903058399085161	2.7099847587255361	10.8353850732375427	F	F	F
14.6612664443506659	3.3663264936155204	11.7805097330318205	F	F	F
16.2903049377237927	0.6512632949439837	10.8353848893587461	F	F	F
16.2902090047378749	5.4106933371214971	14.5873529061470002	T	T	T
14.6891171655501491	2.7035577126449670	13.7082465473305035	T	T	T
16.2903891583086988	3.4027639869952950	14.7474276553252039	T	T	T
14.6772278750563583	0.6864277521169757	13.6525477179688597	T	T	T
14.7081009464211281	5.6235533875532742	17.4523522777542190	T	T	T
16.2903658519629353	2.7931484832391744	16.7247512082600913	T	T	T
14.5155349373261444	3.5632065435282940	17.4836538074457231	T	T	T
16.2901822986170721	0.7984521368403091	16.4056301232248103	T	T	T
0.0000878715693368	0.8603121015591866	19.6072640193508363	T	T	T
1.3702222828589632	2.2213567373201384	21.4817635108467968	T	T	T
0.0001209594718652	0.8669034104010025	23.3106130951906430	T	T	T
0.0001382346109080	3.5631394457888206	19.6575980363239893	T	T	T
1.3672360735730344	4.9345341963962532	21.4808600296529022	T	T	T
0.0001214804418006	3.5791963079714284	23.3288875449870545	T	T	T
2.7163712975405909	0.8746065676230059	19.6293273392459398	T	T	T
4.0777018268396201	2.2528715410070839	21.4236018026871164	T	T	T
2.7428221142443618	0.8683524986720673	23.2997045473702435	T	T	T
2.6486749095868136	3.5682461661744429	19.5326630708276667	T	T	T
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2.7348274992744330	3.5872890738929812	23.3104808382853612	T	T	T
5.4296815386748793	0.8836684817131796	19.6189806738981609	T	T	T
6.7852972942601220	2.2703839830056807	21.4000589939561223	T	T	T

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  5.4467416698209270  0.8731457103428315 23.2546349528783587   T   T   T
  5.3741981497144939  3.5750942781067283 19.4615214574722692   T   T   T
  6.7852711641789405  4.9138698505942910 21.3733924843774297   T   T   T
  5.4377494107385633  3.6008062618190992 23.2893575120440772   T   T   T
  8.1453986180727878  0.8882198088506330 19.6188988570924572   T   T   T
  9.5053758916956177  2.2703183296299150 21.4001272751234062   T   T   T
  8.1452767925109075  0.8753757771675486 23.2360749434022686   T   T   T
  8.1453687335921501  3.5755620671788115 19.4457220146757450   T   T   T
  9.5054294299754556  4.9138629235110880 21.3734871802988948   T   T   T
  8.1452378673710353  3.6074814000613280 23.2750653848132139   T   T   T
 10.8610106318156152  0.8836779284393571 19.6189866597658948   T   T   T
 12.2128758311900398  2.2529270248399360 21.4235706618862629   T   T   T
 10.8439539981668389  0.8732015368042630 23.2547258184321102   T   T   T
 10.9164509746569802  3.5750908220315289 19.4615120976064127   T   T   T
 12.2164734281508327  4.9206638483049545 21.4109341874178973   T   T   T
 10.8528491149491497  3.6008321550552238 23.2894889043304509   T   T   T
 13.5742938170848699  0.8746394057082936 19.6293786346526105   T   T   T
 14.9203627733300852  2.2213781652180589 21.4817568235484231   T   T   T
 13.5478529839307296  0.8683883271143913 23.2996945129041499   T   T   T
 13.6420173011212285  3.5683136693946254 19.5326529774933171   T   T   T
 14.9233780762374906  4.9344940261352201 21.4809114680181956   T   T   T
 13.5558074255206744  3.5872761770745663 23.3105011701952378   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_6x2/Ir E_tot= -359.15361912 eV
 D3-zero damping= -12.9263336 eV, D3-BJ damping= -14.0784276 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
    16.2903792873000057    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4301264291000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.1312880290811052
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2
Selective dynamics
Cartesian
  3.2579958417876056  5.4250480286694351  8.9451241821253618   F   F   F
  1.6289599139581354  2.7099848331968222  8.0000001838787966   F   F   F
  3.2579963758602881  3.3663265680868064  8.9451248436730744   F   F   F
  1.6289590117734154  0.6512633694152701  8.0000000000000000   F   F   F
  1.6289624804379781  5.4250479541981491 11.7805090714841079   F   F   F
  3.2580024100685101  2.7099847587255361 10.8353850732375427   F   F   F
  1.6289630145106604  3.3663264936155204 11.7805097330318205   F   F   F
  3.2580015078837898  0.6512632949439837 10.8353848893587461   F   F   F
  3.2580611387056244  5.3497131648816039 14.5308520923018119   T   T   T
  1.6289240021813018  2.6810268902730958 13.6773968506953185   T   T   T
  3.2578611544121530  3.3536275939617242 14.6052151099532992   T   T   T
  1.6289088085143908  0.6580195540735934 13.6681691668392951   T   T   T
  1.6290120064819540  5.1376474125355038 17.0462974722189280   T   T   T
  3.2582117516078464  2.6266530627513593 16.5805255602087946   T   T   T
  1.6289997297647132  3.3009997857667157 17.3831044353115267   T   T   T
  3.2577615568751517  0.6154960309087375 16.4752172585026386   T   T   T
  6.5160716992476067  5.4250480286694351  8.9451241821253618   F   F   F
  4.8870357714181374  2.7099848331968222  8.0000001838787966   F   F   F
  6.5160722333202896  3.3663265680868064  8.9451248436730744   F   F   F
  4.8870348692334167  0.6512633694152701  8.0000000000000000   F   F   F
  4.8870383378979794  5.4250479541981491 11.7805090714841079   F   F   F
  6.5160782675285107  2.7099847587255361 10.8353850732375427   F   F   F
  4.8870388719706632  3.3663264936155204 11.7805097330318205   F   F   F
  6.5160773653437909  0.6512632949439837 10.8353848893587461   F   F   F
  6.5160848612299667  5.3507139437062676 14.5307074003788124   T   T   T
  4.8870520417449255  2.6817021131423262 13.6774025294278072   T   T   T
  6.5159844248905827  3.3544455416370194 14.6050431085862229   T   T   T
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  4.8869013625879605  0.6586393277774286 13.6680308032631697   T   T   T
  4.8871058561518668  5.1394271115820800 17.0469403634927694   T   T   T
  6.5162804104516914  2.6281047370813098 16.5803818895261657   T   T   T
  4.8870383879359327  3.3024130051218044 17.3830516829890520   T   T   T
  6.5158878451615143  0.6166267450360228 16.4751589468593949   T   T   T
  9.7741475567076090  5.4250480286694351  8.9451241821253618   F   F   F
  8.1451116288781371  2.7099848331968222  8.0000001838787966   F   F   F
  9.7741480907802902  3.3663265680868064  8.9451248436730744   F   F   F
  8.1451107266934173  0.6512633694152701  8.0000000000000000   F   F   F
  8.1451141953579818  5.4250479541981491 11.7805090714841079   F   F   F
  9.7741541249885131  2.7099847587255361 10.8353850732375427   F   F   F
  8.1451147294306629  3.3663264936155204 11.7805097330318205   F   F   F
  9.7741532228037933  0.6512632949439837 10.8353848893587461   F   F   F
  9.7741587541613448  5.3507061423862003 14.5307548153766728   T   T   T
  8.1451407748642080  2.6822899387100900 13.6776051860525936   T   T   T
  9.7743243625194776  3.3544292176082298 14.6050621798753895   T   T   T
  8.1451305098032218  0.6590981239628074 13.6680258333344735   T   T   T
  8.1451212281959826  5.1403070577117447 17.0469071477910461   T   T   T
  9.7740652827827699  2.6280802135657391 16.5804079791462229   T   T   T
  8.1451672618222339  3.3032293429078594 17.3830152626967056   T   T   T
  9.7743740079644610  0.6166080129729590 16.4751826512058912   T   T   T
 13.0322234141676105  5.4250480286694351  8.9451241821253618   F   F   F
 11.4031874863381404  2.7099848331968222  8.0000001838787966   F   F   F
 13.0322239482402935  3.3663265680868064  8.9451248436730744   F   F   F
 11.4031865841534206  0.6512633694152701  8.0000000000000000   F   F   F
 11.4031900528179833  5.4250479541981491 11.7805090714841079   F   F   F
 13.0322299824485164  2.7099847587255361 10.8353850732375427   F   F   F
 11.4031905868906662  3.3663264936155204 11.7805097330318205   F   F   F
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 13.0321308757056205  5.3496718117113353 14.5308440982708937   T   T   T
 11.4031926992935091  2.6816625216265875 13.6773593904712740   T   T   T
 13.0323745698978133  3.3535978965885569 14.6051978383505485   T   T   T
 11.4033107706883339  0.6586186637257943 13.6680114664161110   T   T   T
 11.4031481810377269  5.1393820143277686 17.0470187228025161   T   T   T
 13.0321168564120633  2.6266914601901141 16.5805141103739118   T   T   T
 11.4032918152584735  3.3023708165597432 17.3831624935809224   T   T   T
 13.0324520851947590  0.6155115173595528 16.4752018659366364   T   T   T
 16.2902992716276138  5.4250480286694351  8.9451241821253618   F   F   F
 14.6612633437981401  2.7099848331968222  8.0000001838787966   F   F   F
 16.2902998057002932  3.3663265680868064  8.9451248436730744   F   F   F
 14.6612624416134203  0.6512633694152701  8.0000000000000000   F   F   F
 14.6612659102779848  5.4250479541981491 11.7805090714841079   F   F   F
 16.2903058399085161  2.7099847587255361 10.8353850732375427   F   F   F
 14.6612664443506659  3.3663264936155204 11.7805097330318205   F   F   F
 16.2903049377237927  0.6512632949439837 10.8353848893587461   F   F   F
 16.2903098099858106  5.3491292893660578 14.5306052386563387   T   T   T
 14.6612985647419407  2.6809971012773546 13.6773905128521491   T   T   T
 16.2902959008668056  3.3531116667555465 14.6054084095210523   T   T   T
 14.6613092164978287  0.6579951127738317 13.6681604001616464   T   T   T
 14.6611971761793392  5.1376657544063100 17.0463000087762815   T   T   T
 16.2903505274819942  2.6258139511547154 16.5807665414679235   T   T   T
 14.6613325990257160  3.3010133888123971 17.3830986699055288   T   T   T
 16.2902915985130043  0.6147604425609916 16.4750152722646277   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_6x2/Ir E_tot= -301.89156864 eV
 D3-zero damping= -14.8856557 eV, D3-BJ damping= -16.1345943 eV
Ir
 1.0000000000000000
    16.2903792873000057    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4301264291000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9359299014895974
  36
Cartesian
```

```
 -0.0000000385136031  0.0000000045587058  8.1196752808544304
  1.3574953222012758  1.3575316175216829  9.9731225781779393
 -0.0000000048963670  0.0000000045587058 11.8263986456956793
  0.0000000000000000  2.7150632099912952  8.1196752854131358
  1.3574953002067576  4.0725948040351856  9.9731226036883474
 -0.0000000181293555  2.7150632099912952 11.8263986456956793
  2.7151915626142724  0.0000000047342823  8.1197506967168263
  4.0725948515751984  1.3575316145353762  9.9731235378868917
  2.7151700370286846  0.0000000263776476 11.8265745964314704
  2.7151915926291688  2.7150632098157188  8.1197507116977832
  4.0725948095475806  4.0725948080643084  9.9731235378868917
  2.7151700225773001  2.7150631881723535 11.8265745665056983
  5.4299980819553086  0.0000000035140098  8.1197506891736833
  6.7876943676866750  1.3575316155574075  9.9731225992935979
  5.4300196543243153  0.0000000035140098 11.8265745842955123
  5.4299980940912640  2.7150632110359920  8.1197507031099487
  6.7876943770119009  4.0725948135425947  9.9731226078814270
  5.4300196279125510  2.7150631967601839 11.8265745738732537
  8.1451896786495936 -0.0000000000000000  8.1196752871258582
  9.5026849575262631  1.3575315911440353  9.9731226481953428
  8.1451896918465927 -0.0000000047342823 11.8263986477957825
  8.1451896643737882  2.7150632145500007  8.1196752926382558
  9.5026849507271454  4.0725948258541269  9.9731226313251060
  8.1451896557518424  2.7150632192842825 11.8263986476725389
 10.8603811988967109 -0.0000000054782849  8.1197507438525331
 12.2177844593791534  1.3575316006514460  9.9731235427832576
 10.8603596681897017 -0.0000000054782849 11.8265745739578261
 10.8603811855404846  2.7150632057524775  8.1197507645763185
 12.2177844380753218  4.0725948209054232  9.9731235570590666
 10.8603596643361531  2.7150632200282856 11.8265745739578261
 13.5751877104099279  0.0000000000000000  8.1197507406906517
 14.9328839627870487  1.3575316175216829  9.9731225882004608
 13.5752092590688385 -0.0000000000000000 11.8265745637130237
 13.5751877104099279  2.7150632145500007  8.1197507331475212
 14.9328839818293861  4.0725948258541269  9.9731225825989380
 13.5752092372498971  2.7150632219175583 11.8265745582347410

Interface: ZnO(10-10)/fcc(100)_6x2/Rh E_tot= -620.73802872 eV
 D3-zero damping= -31.5043607 eV, D3-BJ damping= -33.56113 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Rh
 1.0000000000000000
    16.0659761716800027    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3553253905600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.3241942887299736
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2  36
Selective dynamics
Cartesian
  3.2131163208949198  5.3503169460745283  8.9451241821253618   F   F   F
  1.6065206770646594  2.6726542696091213  8.0000001838787966   F   F   F
  3.2131168476106482  3.3199547705521724  8.9451248436730744   F   F   F
  1.6065197873077079  0.6422920909319076  8.0000000000000000   F   F   F
  1.6065232081907475  5.3503168726290991 11.7805090714841079   F   F   F
  3.2131227986964883  2.6726541961636912 10.8353850732375427   F   F   F
  1.6065237349064756  3.3199546971067431 11.7805097330318205   F   F   F
  3.2131219089395362  0.6422920174864777 10.8353848893587461   F   F   F
  3.1922988918663302  5.3153077348794255 14.6028519921266771   T   T   T
  1.5898831730961931  2.6655715119943375 13.6976335175355786   T   T   T
  3.2102288398231926  3.3213222930137163 14.6745487193314457   T   T   T
  1.5967014184544903  0.6632771969127363 13.6570985892766785   T   T   T
  1.5472634796576739  5.4811941620744511 17.5288722488771924   T   T   T
```

3.2225008222728531	2.6673625682199513	16.5885103690885138	T	T	T
1.6647877827092843	3.4594544494272470	17.5428453174389247	T	T	T
3.1595489345366299	0.6927232176339595	16.4536896012384979	T	T	T
6.4263115552309200	5.3503169460745283	8.9451241821253618	F	F	F
4.8197159114006602	2.6726542696091213	8.0000001838787966	F	F	F
6.4263120819466488	3.3199547705521724	8.9451248436730744	F	F	F
4.8197150216437086	0.6422920909319076	8.0000000000000000	F	F	F
4.8197184425267485	5.3503168726290991	11.7805090714841079	F	F	F
6.4263180330324889	2.6726541961636912	10.8353850732375427	F	F	F
4.8197189692424773	3.3199546971067431	11.7805097330318205	F	F	F
6.4263171432755364	0.6422920174864777	10.8353848893587461	F	F	F
6.4148806553073925	5.2886781711504280	14.5824960104228047	T	T	T
4.8049852802675259	2.6428069655037278	13.6739744610043026	T	T	T
6.4255298515432431	3.2973000509408554	14.6372239491302771	T	T	T
4.8050536022122259	0.6424996512520883	13.6639433050521806	T	T	T
4.7432901505140945	5.3896410409047970	17.4175302178656963	T	T	T
6.4361476819107812	2.6072081019369961	16.5337977971725216	T	T	T
4.8772582078450908	3.3909411346123086	17.4356769132640927	T	T	T
6.3978115888419111	0.6394243454619423	16.4442611326429713	T	T	T
9.6395067895669211	5.3503169460745283	8.9451241821253618	F	F	F
8.0329111457366587	2.6726542696091213	8.0000001838787966	F	F	F
9.6395073162826481	3.3199547705521724	8.9451248436730744	F	F	F
8.0329102559797079	0.6422920909319076	8.0000000000000000	F	F	F
8.0329136768627496	5.3503168726290991	11.7805090714841079	F	F	F
9.6395132673684891	2.6726541961636912	10.8353850732375427	F	F	F
8.0329142035784766	3.3199546971067431	11.7805097330318205	F	F	F
9.6395123776115383	0.6422920174864777	10.8353848893587461	F	F	F
9.6508040278323950	5.2887112118330863	14.5826827199386155	T	T	T
8.0329653137389929	2.6319143655797990	13.6635196319322514	T	T	T
9.6403098257389548	3.2973066610429473	14.6374736516632868	T	T	T
8.0328973887248711	0.6324230885143769	13.6661818259531209	T	T	T
8.0322718989121036	5.3632592413664293	17.3707804551086156	T	T	T
9.6295168905476274	2.6071127391630378	16.5341102129985273	T	T	T
8.0328521773040240	3.3642842415937246	17.4096692855596373	T	T	T
9.6669975701286752	0.6393553944551845	16.4444765375038031	T	T	T
12.8527020239029213	5.3503169460745283	8.9451241821253618	F	F	F
11.2461063800726624	2.6726542696091213	8.0000001838787966	F	F	F
12.8527025506186519	3.3199547705521724	8.9451248436730744	F	F	F
11.2461054903157098	0.6422920909319076	8.0000000000000000	F	F	F
11.2461089111987498	5.3503168726290991	11.7805090714841079	F	F	F
12.8527085017044911	2.6726541961636912	10.8353850732375427	F	F	F
11.2461094379144786	3.3199546971067431	11.7805097330318205	F	F	F
12.8527076119475403	0.6422920174864777	10.8353848893587461	F	F	F
12.8730175950691752	5.3155464067903440	14.6033419612354880	T	T	T
11.2608009169075149	2.6430555890797276	13.6741377974787337	T	T	T
12.8554581309618143	3.3215202044568550	14.6748841261311807	T	T	T
11.2605050343210227	0.6426558282560297	13.6639665195896693	T	T	T
11.3211616938876674	5.3896724054983824	17.4180143503313261	T	T	T
12.8430399547595133	2.6675388639968651	16.5888734771570903	T	T	T
11.1883558180090894	3.3910069816344426	17.4359552274462395	T	T	T
12.9050273600312160	0.6929206223780612	16.4541426895595535	T	T	T
16.0658972582389232	5.3503169460745283	8.9451241821253618	F	F	F
14.4593016144086608	2.6726542696091213	8.0000001838787966	F	F	F
16.0658977849546503	3.3199547705521724	8.9451248436730744	F	F	F
14.4593007246517100	0.6422920909319076	8.0000000000000000	F	F	F
14.4593041455347500	5.3503168726290991	11.7805090714841079	F	F	F
16.0659037360404895	2.6726541961636912	10.8353850732375427	F	F	F
14.4593046722504770	3.3199546971067431	11.7805097330318205	F	F	F
16.0659028462835387	0.6422920174864777	10.8353848893587461	F	F	F
16.0656083125940228	5.3353651320348492	14.6152122013984140	T	T	T
14.4754841614953005	2.6656420002465677	13.6976796213624574	T	T	T
16.0657407479803709	3.3393677348327855	14.7288087408326547	T	T	T
14.4685127056041569	0.6633269268580323	13.6571700282113611	T	T	T

```
 14.5172490779928030  5.4812652164369986 17.5289992907069312   T   T   T
 16.0657554188987319  2.7203695362999221 16.6707594222039290   T   T   T
 14.4008012374098335  3.4595168015279247 17.5430623822644876   T   T   T
 16.0652772478869750  0.7417119933993334 16.4495021825862189   T   T   T
  0.0001022766445918  0.8980504098359499 19.6329204011078140   T   T   T
  1.3455691066698232  2.2370762505881796 21.4744895225579704   T   T   T
  0.0002334924691053  0.8919521705787398 23.2960643069056204   T   T   T
  0.0001520850998054  3.5595482834584855 19.6337025631817674   T   T   T
  1.3431336732899515  4.9072256900186435 21.4664448014352409   T   T   T
  0.0005867587351520  3.5724526288329077 23.3172563244715860   T   T   T
  2.7002232512444055  0.9136289027502100 19.6565247923872555   T   T   T
  4.0222638088686660  2.2617049424304385 21.4594143763115319   T   T   T
  2.6873572917670177  0.8937909076667054 23.2929114952450824   T   T   T
  2.6405137883576471  3.5631607452497489 19.5604511622984276   T   T   T
  4.0167007980828302  4.8940039089864671 21.4326521363016376   T   T   T
  2.6826737432844796  3.5802679998891227 23.3086390769108682   T   T   T
  5.3725783230404467  0.9242516546118071 19.6705842827424426   T   T   T
  6.6960413896153925  2.2837965886063896 21.4516405397914518   T   T   T
  5.3652406951107841  0.9004509729446947 23.2776393004638749   T   T   T
  5.3130924846612144  3.5670039461271141 19.5067751423582756   T   T   T
  6.6923860620428091  4.8908283581570640 21.4079411734740184   T   T   T
  5.3579589022363256  3.5961649559723208 23.3043345772863084   T   T   T
  8.0335149932332985  0.9260544149073472 19.6812409202835674   T   T   T
  9.3705207836881410  2.2841430164838519 21.4517481643549175   T   T   T
  8.0332133707191815  0.9057082510212988 23.2680701262494907   T   T   T
  8.0332720152854087  3.5588883521422225 19.4917044080379007   T   T   T
  9.3745358535649554  4.8908182737046317 21.4080016132341662   T   T   T
  8.0332743885333713  3.6058292645599606 23.3009143742532423   T   T   T
 10.6944385905912931  0.9250201031149541 19.6709938198244139   T   T   T
 12.0444846879922647  2.2626207244349401 21.4605128016020998   T   T   T
 10.7013517578721782  0.9010192113356168 23.2781366275924739   T   T   T
 10.7536638256528239  3.5674391653162876 19.5073425753475682   T   T   T
 12.0491871100813732  4.8945519521065677 21.4334288601170044   T   T   T
 10.7088224874863389  3.5966555675716552 23.3053717495240349   T   T   T
 13.3660888267973199  0.9140809388696957 19.6574719917748411   T   T   T
 14.7211539796082871  2.2369673565680070 21.4748252204470660   T   T   T
 13.3794293211346087  0.8941609324225808 23.2931372434654520   T   T   T
 13.4259271812948118  3.5641822705468869 19.5612082966624605   T   T   T
 14.7228614144592651  4.9073452764013661 21.4666299266984346   T   T   T
 13.3842088506393786  3.5808873355690198 23.3090179866044060   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_6x2/Rh E_tot= -359.35666997 eV
 D3-zero damping= -13.0756285 eV, D3-BJ damping= -14.3790934 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
    16.0659761716800027    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3553253905600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.1312880290811052
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2
Selective dynamics
Cartesian
  3.2131163208949198  5.3503169460745283  8.9451241821253618   F   F   F
  1.6065206770646594  2.6726542696091213  8.0000001838787966   F   F   F
  3.2131168476106482  3.3199547705521724  8.9451248436730744   F   F   F
  1.6065197873077079  0.6422920909319076  8.0000000000000000   F   F   F
  1.6065232081907475  5.3503168726290991 11.7805090714841079   F   F   F
  3.2131227986964883  2.6726541961636912 10.8353850732375427   F   F   F
  1.6065237349064756  3.3199546971067431 11.7805097330318205   F   F   F
  3.2131219089395362  0.6422920174864777 10.8353848893587461   F   F   F
  3.2131923800653892  5.2980453933855252 14.5703801491265814   T   T   T
```

1.6064845241818877	2.6615239876501993	13.6890499260789351	T	T	T
3.2129783103359832	3.3112164658213583	14.6571644109926691	T	T	T
1.6065264698711603	0.6529017897766013	13.6670118006332828	T	T	T
1.6067970387926067	5.0996180477612967	17.1413066608014333	T	T	T
3.2128500938813609	2.6245666001098886	16.6355330030581889	T	T	T
1.6066397037855318	3.2720028987721643	17.4966381314739081	T	T	T
3.2135830724327601	0.6303620372388818	16.5069148278155815	T	T	T
6.4263115552309200	5.3503169460745283	8.9451241821253618	F	F	F
4.8197159114006602	2.6726542696091213	8.0000001838787966	F	F	F
6.4263120819466488	3.3199547705521724	8.9451248436730744	F	F	F
4.8197150216437086	0.6422920909319076	8.0000000000000000	F	F	F
4.8197184425267485	5.3503168726290991	11.7805090714841079	F	F	F
6.4263180330324889	2.6726541961636912	10.8353850732375427	F	F	F
4.8197189692424773	3.3199546971067431	11.7805097330318205	F	F	F
6.4263171432755364	0.6422920174864777	10.8353848893587461	F	F	F
6.4263772586468555	5.2968739513304062	14.5699933496424414	T	T	T
4.8195084043733107	2.6613873846553107	13.6890693935234982	T	T	T
6.4264070787015308	3.3101004604661544	14.6573005599437671	T	T	T
4.8198886782617087	0.6526253316256316	13.6669365041751956	T	T	T
4.8200139646915430	5.0983892552301997	17.1410628742234437	T	T	T
6.4262703112626811	2.6239101074976108	16.6356637799495566	T	T	T
4.8197315150977449	3.2710736073968145	17.4961405946533048	T	T	T
6.4264708913380559	0.6295518391390413	16.5063169154996245	T	T	T
9.6395067895669211	5.3503169460745283	8.9451241821253618	F	F	F
8.0329111457366587	2.6726542696091213	8.0000001838787966	F	F	F
9.6395073162826481	3.3199547705521724	8.9451248436730744	F	F	F
8.0329102559797079	0.6422920909319076	8.0000000000000000	F	F	F
8.0329136768627496	5.3503168726290991	11.7805090714841079	F	F	F
9.6395132673684891	2.6726541961636912	10.8353850732375427	F	F	F
8.0329142035784766	3.3199546971067431	11.7805097330318205	F	F	F
9.6395123776115383	0.6422920174864777	10.8353848893587461	F	F	F
9.6396553110228016	5.2969281258970069	14.5701397645761617	T	T	T
8.0330187757783200	2.6607069893646140	13.6888772782855437	T	T	T
9.6395223274048316	3.3101451275610896	14.6573907098115299	T	T	T
8.0330129861932154	0.6520771088417610	13.6669480045817515	T	T	T
8.0329867492545475	5.0983661473882131	17.1408090910543720	T	T	T
9.6397664318907488	2.6239666142054894	16.6358741811909070	T	T	T
8.0329440268129026	3.2708448240080812	17.4962282261357345	T	T	T
9.6394946970192112	0.6295982340091126	16.5064456985561314	T	T	T
12.8527020239029213	5.3503169460745283	8.9451241821253618	F	F	F
11.2461063800726624	2.6726542696091213	8.0000001838787966	F	F	F
12.8527025506186519	3.3199547705521724	8.9451248436730744	F	F	F
11.2461054903157098	0.6422920909319076	8.0000000000000000	F	F	F
11.2461089111987498	5.3503168726290991	11.7805090714841079	F	F	F
12.8527085017044911	2.6726541961636912	10.8353850732375427	F	F	F
11.2461094379144786	3.3199546971067431	11.7805097330318205	F	F	F
12.8527076119475403	0.6422920174864777	10.8353848893587461	F	F	F
12.8527211869770710	5.2979403090857167	14.5703551430716178	T	T	T
11.2463267620471488	2.6613736610078069	13.6890318372169215	T	T	T
12.8528976605941594	3.3111442999274665	14.6571237226224085	T	T	T
11.2460641277203059	0.6525962552057318	13.6669379962287820	T	T	T
11.2459577938267703	5.0983976078183932	17.1409828283712926	T	T	T
12.8533204925839506	2.6245589707131431	16.6354947013852090	T	T	T
11.2464082577888398	3.2710536360979079	17.4960721162879764	T	T	T
12.8524357182487563	0.6303326304705392	16.5068794974534327	T	T	T
16.0658972582389232	5.3503169460745283	8.9451241821253618	F	F	F
14.4593016144086608	2.6726542696091213	8.0000001838787966	F	F	F
16.0658977849546503	3.3199547705521724	8.9451248436730744	F	F	F
14.4593007246517100	0.6422920909319076	8.0000000000000000	F	F	F
14.4593041455347500	5.3503168726290991	11.7805090714841079	F	F	F
16.0659037360404895	2.6726541961636912	10.8353850732375427	F	F	F
14.4593046722504770	3.3199546971067431	11.7805097330318205	F	F	F
16.0659028462835387	0.6422920174864777	10.8353848893587461	F	F	F

```
 16.0659658191559274  5.2978136425064610 14.5704706935477990   T   T   T
 14.4594765968772148  2.6615511309240381 13.6890402156048197   T   T   T
 16.0659465467784521  3.3110520676218695 14.6574573407992652   T   T   T
 14.4593785687030714  0.6528736390439595 13.6670116785195415   T   T   T
 14.4592780585078753  5.0995481995032543 17.1411675793380631   T   T   T
 16.0662842233790286  2.6247852585980342 16.6358623002435202   T   T   T
 14.4596951427829126  3.2719862873975627 17.4963188918164114   T   T   T
 16.0660640819347513  0.6304214957355927 16.5068316875625563   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_6x2/Rh E_tot= -248.61830165 eV
 D3-zero damping= -12.0179799 eV, D3-BJ damping= -14.4941094 eV
Rh
 1.0000000000000000
    16.0659761716800027    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3553253905600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9359299014895974
  36
Cartesian
  0.0000000837409559  0.0000000000000002  8.1302341454762708
  1.3393401252264487  1.3388313550660988  9.9735652271360689
  0.0000000477618198  0.0000000000000000 11.8168028072705944
  0.0000000583488020  2.6776626952800004  8.1302342147084019
  1.3393400870560113  4.0164940354938983  9.9735652271360689
  0.0000000143036353  2.6776626952800004 11.8168028853700999
  2.6768189398161448 -0.0000000143036353  8.1286205166771364
  4.0164940519817600  1.3388313421929392  9.9722770145994559
  2.6771490243424214 -0.0000000143036353 11.8172037862717048
  2.6768189070927706  2.6776627095836365  8.1286204799089425
  4.0164940325012699  4.0164940483670613  9.9722770145994559
  2.6771490308394434  2.6776627095836365 11.8172037863820130
  5.3561690714549597  0.0000000129834673  8.1286204921124607
  6.6936480150040785  1.3388313170059702  9.9735652586623651
  5.3558391164260772  0.0000000129834673 11.8172038073143533
  5.3561690714549597  2.6776626822965341  8.1286205109706575
  6.6936480202912376  4.0164940735540311  9.9735652586623651
  5.3558391164260772  2.6776626822965341 11.8172037204966678
  8.0329880709614550 -0.0000000000000000  8.1302341965198686
  9.3723281293888299  1.3388313564965755  9.9735652745281538
  8.0329880689716298  0.0000000000000000 11.8168028707121717
  8.0329880632651527  2.6776626952800004  8.1302342030168955
  9.3723281566759358  4.0164940340634274  9.9735652745281538
  8.0329880494911396  2.6776626952800004 11.8168028854804099
 10.7098070899166142  0.0000000000000000  8.1286206226210069
 12.0494821731680428  1.3388313374806871  9.9722770812126189
 10.7101371532985183  0.0000000076963054 11.8172037793100788
 10.7098070901760334  2.6776626952800004  8.1286206096375420
 12.0494821430636350  4.0164940530793167  9.9722770835721679
 10.7101371615697403  2.6776626875836955 11.8172038425029289
 13.3891571532997560 -0.0000000200101145  8.1286205136930860
 14.7266360794471307  1.3388313374806871  9.9735652835899167
 13.3888271649229793 -0.0000000143036353 11.8172038267021726
 13.3891571389961221  2.6776627009864797  8.1286205036372277
 14.7266360900710573  4.0164940530793167  9.9735652978935487
 13.3888271376358787  2.6776627095836365 11.8172037925461115

Interface: ZnO(10-10)/fcc(100)_6x2/Os E_tot= -742.70836333 eV
 D3-zero damping= -29.3072045 eV, D3-BJ damping= -32.7416084 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Os
 1.0000000000000000
    16.2504856984800057    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4168285661600013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.3241942887299736
```

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   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2  36
Selective dynamics
Cartesian
  3.2500173199743734  5.4117626022488725  8.9451241821253618   F   F   F
  1.6249707461268885  2.7033483381995405  8.0000001838787966   F   F   F
  3.2500178527391630  3.3580827546327026  8.9451248436730744   F   F   F
  1.6249698461515329  0.6496684873922814  8.0000000000000000   F   F   F
  1.6249733063216663  5.4117625279599588 11.7805090714841079   F   F   F
  3.2500238721701828  2.7033482639106272 10.8353850732375427   F   F   F
  1.6249738390864554  3.3580826803437898 11.7805097330318205   F   F   F
  3.2500229721948273  0.6496684131033682 10.8353848893587461   F   F   F
  3.2320491598301362  5.3801274617614574 14.5649502862552325   T   T   T
  1.6006404078480261  2.6946166657105182 13.7032981402036356   T   T   T
  3.2555771646591363  3.3741756922649770 14.6435402274168265   T   T   T
  1.6134287835484173  0.6803424212516479 13.6547967970565676   T   T   T
  1.5661940422130591  5.6050855882897679 17.4920392835330212   T   T   T
  3.3208579894812655  2.7017821500214478 16.5321667755293191   T   T   T
  1.7812611135205625  3.5246218199021166 17.5349426702554609   T   T   T
  3.2107778997379950  0.7181973633562839 16.4058539262347125   T   T   T
  6.5001144596703746  5.4117626022488725  8.9451241821253618   F   F   F
  4.8750678858228902  2.7033483381995405  8.0000001838787966   F   F   F
  6.5001149924351651  3.3580827546327026  8.9451248436730744   F   F   F
  4.8750669858475346  0.6496684873922814  8.0000000000000000   F   F   F
  4.8750704460176681  5.4117625279599588 11.7805090714841079   F   F   F
  6.5001210118661845  2.7033482639106272 10.8353850732375427   F   F   F
  4.8750709787824578  3.3580826803437898 11.7805097330318205   F   F   F
  6.5001201118908281  0.6496684131033682 10.8353848893587461   F   F   F
  6.4893476006657727  5.3521468027628600 14.5463896039007938   T   T   T
  4.8648586248757040  2.6680303124107594 13.6594594938810570   T   T   T
  6.5029509486598238  3.3504171915048100 14.6023439911811010   T   T   T
  4.8631299263139587  0.6610527801277503 13.6567907549882097   T   T   T
  4.8025813694333905  5.4999115155588356 17.3993146881021232   T   T   T
  6.5323367365729776  2.6400822438890659 16.4720538528846774   T   T   T
  4.9949224364997269  3.4476543861177102 17.4374403701050689   T   T   T
  6.4752186340801181  0.6633370734889006 16.3952144923545831   T   T   T
  9.7502115993663772  5.4117626022488725  8.9451241821253618   F   F   F
  8.1251650255188910  2.7033483381995405  8.0000001838787966   F   F   F
  9.7502121321311659  3.3580827546327026  8.9451248436730744   F   F   F
  8.1251641255435345  0.6496684873922814  8.0000000000000000   F   F   F
  8.1251675857136707  5.4117625279599588 11.7805090714841079   F   F   F
  9.7502181515621853  2.7033482639106272 10.8353850732375427   F   F   F
  8.1251681184784577  3.3580826803437898 11.7805097330318205   F   F   F
  9.7502172515868306  0.6496684131033682 10.8353848893587461   F   F   F
  9.7611866758701815  5.3521120832007876 14.5463935009285272   T   T   T
  8.1252709222654520  2.6555614109170653 13.6485177068821226   T   T   T
  9.7475686638716521  3.3503734457923362 14.6024113122902026   T   T   T
  8.1252656038908437  0.6502577226155465 13.6594716774688720   T   T   T
  8.1251219842315496  5.4591053256794000 17.3355193875112192   T   T   T
  9.7178064566145039  2.6400673748111108 16.4720318700878359   T   T   T
  8.1250827652244819  3.4117493619824120 17.4120583576245949   T   T   T
  9.7750085196938823  0.6633645010982033 16.3952470042556584   T   T   T
 13.0003087390623779  5.4117626022488725  8.9451241821253618   F   F   F
 11.3752621652148935  2.7033483381995405  8.0000001838787966   F   F   F
 13.0003092718271684  3.3580827546327026  8.9451248436730744   F   F   F
 11.3752612652395371  0.6496684873922814  8.0000000000000000   F   F   F
 11.3752647254096715  5.4117625279599588 11.7805090714841079   F   F   F
 13.0003152912581896  2.7033482639106272 10.8353850732375427   F   F   F
 11.3752652581744602  3.3580826803437898 11.7805097330318205   F   F   F
 13.0003143912828332  0.6496684131033682 10.8353848893587461   F   F   F
 13.0184830304918915  5.3801518035649689 14.5651604522754816   T   T   T
 11.3856619824356624  2.6680849543665972 13.6593419511427374   T   T   T
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12.9947896531706331	3.3741935428789174	14.6436888034036006	T	T	T
11.3873971852118903	0.6610318591334976	13.6568221199555708	T	T	T
11.4472523136845545	5.4998427725592336	17.3995594989469566	T	T	T
12.9295598085220558	2.7019526142628894	16.5324856315358595	T	T	T
11.2552644127536663	3.4475597613453357	17.4375242915094475	T	T	T
13.0389755312709426	0.7183913407635338	16.4059779474156322	T	T	T
16.2504058787583823	5.4117626022488725	8.9451241821253618	F	F	F
14.6253593049108925	2.7033483381995405	8.0000001838787966	F	F	F
16.2504064115231692	3.3580827546327026	8.9451248436730744	F	F	F
14.6253584049355378	0.6496684873922814	8.0000000000000000	F	F	F
14.6253618651056723	5.4117625279599588	11.7805090714841079	F	F	F
16.2504124309541886	2.7033482639106272	10.8353850732375427	F	F	F
14.6253623978704610	3.3580826803437898	11.7805097330318205	F	F	F
16.2504115309788304	0.6496684131033682	10.8353848893587461	F	F	F
16.2504506434886835	5.3928039566320516	14.5861536600000381	T	T	T
14.6496353860177209	2.6944848667021128	13.7033621750911028	T	T	T
16.2503849366844655	3.3853469030076710	14.7526394796611147	T	T	T
14.6369452362259143	0.6803091462879520	13.6547351710973874	T	T	T
14.6833297824751927	5.6055607454257945	17.4922340429866061	T	T	T
16.2504347665291853	2.7663392899894097	16.7086174354675734	T	T	T
14.4692027930977680	3.5249528458520092	17.5353446266619528	T	T	T
16.2500833731676018	0.7737267527128096	16.4070252642550010	T	T	T
-0.0005028495693975	0.9189008115677338	19.6430493157713819	T	T	T
1.3618948682002505	2.2807834332041241	21.4788224165757775	T	T	T
-0.0002376545918431	0.9340565970848087	23.3142026017763406	T	T	T
-0.0004631048208315	3.6254236767216703	19.6577341506398291	T	T	T
1.3630075207798196	4.9514561440172153	21.4926809836989605	T	T	T
0.0000080286875554	3.6381817805424905	23.3407597484141043	T	T	T
2.7204406732360278	0.9416069752609841	19.6614577978820613	T	T	T
4.0438327350581140	2.3564574580050008	21.4463337711969686	T	T	T
2.7459520913764233	0.9496230249387000	23.3015830746350829	T	T	T
2.6142061361506221	3.6261358845866218	19.5439653262583519	T	T	T
4.0548556420981834	4.9516895961305822	21.4143143926634210	T	T	T
2.7282853358678514	3.6640446131983331	23.3500798411681778	T	T	T
5.4136148966917279	0.9855619704794025	19.6852145484197933	T	T	T
6.7730602722797331	2.4101564525612900	21.4470645730685519	T	T	T
5.4585302716954480	0.9799565871900633	23.2781764412352459	T	T	T
5.3492345955295058	3.6433254598115861	19.5071848079976462	T	T	T
6.7634738393779825	4.9790685598598481	21.3698380710960727	T	T	T
5.4213721102816868	3.7102669897668736	23.3185805333231606	T	T	T
8.1248278103490463	0.9974514394771614	19.6832360840893799	T	T	T
9.4767064136026260	2.4100942394025848	21.4469836394232090	T	T	T
8.1250655590197116	0.9896855487600481	23.2687146697397509	T	T	T
8.1249057367364443	3.6488283489640745	19.4911226513213194	T	T	T
9.4863060228267617	4.9791231996272822	21.3699151372044902	T	T	T
8.1249643828750315	3.7354913436409154	23.3139260315345318	T	T	T
10.8360923623533232	0.9855409114446633	19.6853229985066385	T	T	T
12.2058918790859110	2.3565224917999918	21.4464397818202066	T	T	T
10.7912026777016514	0.9798848664236680	23.2782436537916269	T	T	T
10.9007024559551269	3.6433957490578677	19.5073346193102708	T	T	T
12.1949587849082182	4.9517507873544924	21.4143930779619645	T	T	T
10.8284063289178238	3.7102132028173376	23.3185966925501340	T	T	T
13.5292776965426000	0.9417676211981271	19.6616826139621388	T	T	T
14.8878305613215982	2.2809107719564441	21.4790664852477846	T	T	T
13.5041081671246577	0.9494354714036960	23.3017441791970015	T	T	T
13.6356042169855058	3.6263685991631687	19.5442607826473456	T	T	T
14.8869548642220799	4.9514323334462702	21.4932343552479601	T	T	T
13.5213523940279590	3.6643503228450141	23.3502565580879811	T	T	T

Oxide reference: ZnO(10-10)/fcc(100)_6x2/Os E_tot= -359.22433165 eV
D3-zero damping= -12.95048 eV, D3-BJ damping= -14.1292757 eV
Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn O Zn
O Zn O Zn O Zn O Zn O Zn O Zn O Zn O

```
 1.0000000000000000
    16.2504856984800057    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4168285661600013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.1312880290811052
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2
Selective dynamics
Cartesian
  3.2500173199743734  5.4117626022488725  8.9451241821253618   F   F   F
  1.6249707461268885  2.7033483381995405  8.0000001838787966   F   F   F
  3.2500178527391630  3.3580827546327026  8.9451248436730744   F   F   F
  1.6249698461515329  0.6496684873922814  8.0000000000000000   F   F   F
  1.6249733063216663  5.4117625279599588 11.7805090714841079   F   F   F
  3.2500238721701828  2.7033482639106272 10.8353850732375427   F   F   F
  1.6249738390864554  3.3580826803437898 11.7805097330318205   F   F   F
  3.2500229721948273  0.6496684131033682 10.8353848893587461   F   F   F
  3.2499502226628274  5.3393214039901737 14.5392026499045723   T   T   T
  1.6249658584253588  2.6769327744915135 13.6787163265916405   T   T   T
  3.2500460482822531  3.3433342822151997 14.6144189905057829   T   T   T
  1.6249447024946686  0.6561226308787708 13.6688480418288023   T   T   T
  1.6248345403410331  5.1277640618001001 17.0658536703047865   T   T   T
  3.2499305172219812  2.6233523343411029 16.5900422644705543   T   T   T
  1.6247992633175776  3.2921692808338165 17.4038826681257675   T   T   T
  3.2496530871338010  0.6151686309551776 16.4826315551655753   T   T   T
  6.5001144596703746  5.4117626022488725  8.9451241821253618   F   F   F
  4.8750678858228902  2.7033483381995405  8.0000001838787966   F   F   F
  6.5001149924351651  3.3580827546327026  8.9451248436730744   F   F   F
  4.8750669858475346  0.6496684873922814  8.0000000000000000   F   F   F
  4.8750704460176681  5.4117625279599588 11.7805090714841079   F   F   F
  6.5001210118661845  2.7033482639106272 10.8353850732375427   F   F   F
  4.8750709787824578  3.3580826803437898 11.7805097330318205   F   F   F
  6.5001201118908281  0.6496684131033682 10.8353848893587461   F   F   F
  6.5000718137414184  5.3396579381910092 14.5392807971771898   T   T   T
  4.8750548358687542  2.6769811310353080 13.6786812609259325   T   T   T
  6.5000663503904628  3.3436492345729953 14.6144011618975949   T   T   T
  4.8749552559455251  0.6561904774752778 13.6689072682206838   T   T   T
  4.8748152489978152  5.1285806257220754 17.0659736430002766   T   T   T
  6.4999029622046489  2.6239175186001957 16.5900072125766265   T   T   T
  4.8748078604904048  3.2929481151889517 17.4038996656997220   T   T   T
  6.4998847545474465  0.6157055641382322 16.4828484417427141   T   T   T
  9.7502115993663772  5.4117626022488725  8.9451241821253618   F   F   F
  8.1251650255188910  2.7033483381995405  8.0000001838787966   F   F   F
  9.7502121321311659  3.3580827546327026  8.9451248436730744   F   F   F
  8.1251641255435345  0.6496684873922814  8.0000000000000000   F   F   F
  8.1251675857136707  5.4117625279599588 11.7805090714841079   F   F   F
  9.7502181515621853  2.7033482639106272 10.8353850732375427   F   F   F
  8.1251681184784577  3.3580826803437898 11.7805097330318205   F   F   F
  9.7502172515868306  0.6496684131033682 10.8353848893587461   F   F   F
  9.7501356449544136  5.3396500290263038 14.5393238777257015   T   T   T
  8.1251641789921614  2.6772762610728837 13.6787842164629527   T   T   T
  9.7502106563071553  3.3436547786825495 14.6143975125637926   T   T   T
  8.1251110886325275  0.6563755440169150 13.6689168005453823   T   T   T
  8.1249756411565279  5.1288038506019511 17.0661433232043755   T   T   T
  9.7499135048002508  2.6239315115378949 16.5900386816882772   T   T   T
  8.1249385780514150  3.2932059719997069 17.4039598697048099   T   T   T
  9.7500949936581911  0.6156887305925611 16.4828695245075885   T   T   T
 13.0003087390623779  5.4117626022488725  8.9451241821253618   F   F   F
 11.3752621652148935  2.7033483381995405  8.0000001838787966   F   F   F
 13.0003092718271684  3.3580827546327026  8.9451248436730744   F   F   F
 11.3752612652395371  0.6496684873922814  8.0000000000000000   F   F   F
 11.3752647254096715  5.4117625279599588 11.7805090714841079   F   F   F
 13.0003152912581896  2.7033482639106272 10.8353850732375427   F   F   F
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 11.3752652581744602  3.3580826803437898 11.7805097330318205   F   F   F
 13.0003143912828332  0.6496684131033682 10.8353848893587461   F   F   F
 13.0003332255012438  5.3393351177887389 14.5392272427955564   T   T   T
 11.3753159082072628  2.6770127606606993 13.6787578243262153   T   T   T
 13.0002906819408768  3.3433266557233408 14.6144419183452090   T   T   T
 11.3752767008005460  0.6561888204725214 13.6689196349228652   T   T   T
 11.3751305955336530  5.1285810631083244 17.0660313325979693   T   T   T
 12.9999487297062295  2.6233450032705914 16.5900936176174163   T   T   T
 11.3750654990369338  3.2929444091620979 17.4039458984491056   T   T   T
 13.0003558644693200  0.6151362973811684 16.4826815322552527   T   T   T
 16.2504058787583823  5.4117626022488725  8.9451241821253618   F   F   F
 14.6253593049108925  2.7033483381995405  8.0000001838787966   F   F   F
 16.2504064115231692  3.3580827546327026  8.9451248436730744   F   F   F
 14.6253584049355378  0.6496684873922814  8.0000000000000000   F   F   F
 14.6253618651056723  5.4117625279599588 11.7805090714841079   F   F   F
 16.2504124309541886  2.7033482639106272 10.8353850732375427   F   F   F
 14.6253623978704610  3.3580826803437898 11.7805097330318205   F   F   F
 16.2504115309788304  0.6496684131033682 10.8353848893587461   F   F   F
 16.2504418803764494  5.3393121119402327 14.5392701560699216   T   T   T
 14.6254648589874687  2.6769130245653328 13.6787295377503249   T   T   T
 16.2504291006196944  3.3433437791109659 14.6143919815156913   T   T   T
 14.6253217229308490  0.6560900593923560 13.6688686416305973   T   T   T
 14.6252026283564760  5.1277516865433883 17.0658806564790595   T   T   T
 16.2501727774404685  2.6229569656030067 16.5899197394161746   T   T   T
 14.6251096242142040  3.2921366517206212 17.4039045170340323   T   T   T
 16.2502567117492625  0.6148361617884304 16.4827709377503346   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_6x2/Os E_tot= -370.48664251 eV
 D3-zero damping= -11.5652314 eV, D3-BJ damping= -13.8621093 eV
Os
 1.0000000000000000
    16.2504856984800057    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4168285661600013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9359299014895974
  36
Cartesian
  0.0000000000000000  0.0000000000000000  8.1220335790683951
  1.3549205879341681  1.3542071676208884  9.9732319511788337
  0.0000000064043246  0.0000000000000000 11.8239654978100415
 -0.0000000484319961  2.7084142830800007  8.1220336034044180
  1.3549206113746692  4.0626213985391120  9.9732319511788337
  0.0000000064043246  2.7084142830800007 11.8239654978100415
  2.7077537987414790 -0.0000000234405018  8.1216049851755923
  4.0626214042879658  1.3542071365388701  9.9737780796349753
  2.7079144526978203 -0.0000000000000000 11.8243210942261943
  2.7077538496264646  2.7084142830800007  8.1216049654990297
  4.0626214286239852  4.0626214296211307  9.9737780796349753
  2.7079144500574341  2.7084143065205026 11.8243211185622137
  5.4174890473900579  0.0000000000000000  8.1216050132755502
  6.7703222555569829  1.3542071415400003  9.9732319796204649
  5.4173283934337180 -0.0000000000000000 11.8243210922071214
  5.4174889996135347  2.7084142830800007  8.1216049871946598
  6.7703222352249472  4.0626214246200014  9.9732319796204649
  5.4173283960741045  2.7084142830800007 11.8243211203070828
  8.1252428492400028 -0.0000000000000000  8.1220336067870793
  9.4801634835871020  1.3542071415400003  9.9732319320218892
  8.1252428581830127 -0.0000000000000000 11.8239655435674997
  8.1252428492400028  2.7084142830800007  8.1220336027830999
  9.4801634835871020  4.0626213961783701  9.9732319320218892
  8.1252428689165690  2.7084142830800007 11.8239655435674997
 10.8329967296068119  0.0000000000000000  8.1216050121861567
 12.1878642796088528  1.3542071357911494  9.9737780693189180
 10.8331573195437798 -0.0000000477765225 11.8243210748913015
```

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 10.8329967296068119  2.7084142830800007  8.1216050406277880
 12.1878642714992615  4.0626214500454152  9.9737780693189180
 10.8331572691268718  2.7084142830800007 11.8243210788952862
 13.5427318658897171 -0.0000000000000000  8.1216049858310644
 14.8955650651300555  1.3542071421954740  9.9732319401150509
 13.5425712643693519  0.0000000000000000 11.8243211038867777
 13.5427318462131492  2.7084142830800007  8.1216049858310644
 14.8955650651300555  4.0626214239645257  9.9732319401150509
 13.5425712380142613  2.7084142830800007 11.8243211119963743

Interface: ZnO(10-10)/fcc(100)_6x2/Ru E_tot= -680.65168004 eV
 D3-zero damping= -30.8903779 eV, D3-BJ damping= -33.0291739 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Ru
 1.0000000000000000
    15.9971684516400039    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3323894838800010    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.3241942887299736
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2  36
Selective dynamics
Cartesian
  3.1993551148591606  5.3274024896719538  8.9451241821253618   F   F   F
  1.5996402345814453  2.6612077664659672  8.0000001838787966   F   F   F
  3.1993556393190592  3.3057359944282361  8.9451248436730744   F   F   F
  1.5996393486351645  0.6395412680809034  8.0000000000000000   F   F   F
  1.5996427548671703  5.3274024165410783 11.7805090714841079   F   F   F
  3.1993615649174565  2.6612076933350908 10.8353850732375427   F   F   F
  1.5996432793270685  3.3057359212973605 11.7805097330318205   F   F   F
  3.1993606789711753  0.6395411949500270 10.8353848893587461   F   F   F
  3.1812205823848783  5.3127576271302006 14.6138670239958905   T   T   T
  1.5865951366854332  2.6667023776591465 13.7001579595202667   T   T   T
  3.1971306157663064  3.3186608979509318 14.7015161765183731   T   T   T
  1.5924447907332444  0.6691537663934901 13.6536955535277222   T   T   T
  1.5369917473207868  5.5139474972587603 17.5682296677221927   T   T   T
  3.2236235605463794  2.6824356693280711 16.6083994897796217   T   T   T
  1.6536228025094846  3.4539454497262621 17.6087654044442417   T   T   T
  3.1425510903211227  0.7065891891333291 16.4598700003501897   T   T   T
  6.3987888051871611  5.3274024896719538  8.9451241821253618   F   F   F
  4.7990739249094467  2.6612077664659672  8.0000001838787966   F   F   F
  6.3987893296470606  3.3057359944282361  8.9451248436730744   F   F   F
  4.7990730389631659  0.6395412680809034  8.0000000000000000   F   F   F
  4.7990764451951717  5.3274024165410783 11.7805090714841079   F   F   F
  6.3987952552454574  2.6612076933350908 10.8353850732375427   F   F   F
  4.7990769696550704  3.3057359212973605 11.7805097330318205   F   F   F
  6.3987943692991767  0.6395411949500270 10.8353848893587461   F   F   F
  6.3884199525233063  5.2811179302321865 14.6038723677043638   T   T   T
  4.7874675648385061  2.6433970944698406 13.6800533804618212   T   T   T
  6.3993198122162926  3.2892688612325411 14.6676454524341686   T   T   T
  4.7875828290469418  0.6464955920752009 13.6631592282873680   T   T   T
  4.7146913780743080  5.4217746587370383 17.4790797694426523   T   T   T
  6.4176023636757851  2.6160439782727050 16.5616903695945368   T   T   T
  4.8691343883129248  3.3897419666794479 17.5091286768252345   T   T   T
  6.3680715603369320  0.6460060441128976 16.4612834810499571   T   T   T
  9.5982224955151629  5.3274024896719538  8.9451241821253618   F   F   F
  7.9985076152374459  2.6612077664659672  8.0000001838787966   F   F   F
  9.5982230199750607  3.3057359944282361  8.9451248436730744   F   F   F
  7.9985067292911651  0.6395412680809034  8.0000000000000000   F   F   F
  7.9985101355231736  5.3274024165410783 11.7805090714841079   F   F   F
  9.5982289455734584  2.6612076933350908 10.8353850732375427   F   F   F
  7.9985106599830704  3.3057359212973605 11.7805097330318205   F   F   F
  9.5982280596271767  0.6395411949500270 10.8353848893587461   F   F   F
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9.6078107402816073	5.2809060810802109	14.6033984830567825	T	T	T
7.9980362326493637	2.6302145749850654	13.6690164234499001	T	T	T
9.5968701269207504	3.2891543425130236	14.6674097981113700	T	T	T
7.9980626591550950	0.6335711963774805	13.6668038432587480	T	T	T
7.9979038957101700	5.3831094320398263	17.4367220707425510	T	T	T
9.5783990562003947	2.6159571299033773	16.5614561366947051	T	T	T
7.9982147829471915	3.3505107510835170	17.5004765373744249	T	T	T
9.6276293047124053	0.6458783400997850	16.4608396209289225	T	T	T
12.7976561858431630	5.3274024896719538	8.9451241821253618	F	F	F
11.1979413055654486	2.6612077664659672	8.0000001838787966	F	F	F
12.7976567103030643	3.3057359944282361	8.9451248436730744	F	F	F
11.1979404196191688	0.6395412680809034	8.0000000000000000	F	F	F
11.1979438258511745	5.3274024165410783	11.7805090714841079	F	F	F
12.7976626359014620	2.6612076933350908	10.8353850732375427	F	F	F
11.1979443503110723	3.3057359212973605	11.7805097330318205	F	F	F
12.7976617499551804	0.6395411949500270	10.8353848893587461	F	F	F
12.8154558331000619	5.3127029140990780	14.6135493995883117	T	T	T
11.2089189634901789	2.6433139135023831	13.6800089395514064	T	T	T
12.7993850237530591	3.3186555708156296	14.7008724046812755	T	T	T
11.2088887168859337	0.6464561926463346	13.6631487090039183	T	T	T
11.2810338114363145	5.4220301170601868	17.4775193579769912	T	T	T
12.7730035784931193	2.6819957354391062	16.6074679036072368	T	T	T
11.1278382590599811	3.3895503493687640	17.5065732954482485	T	T	T
12.8543939888424745	0.7062715239751418	16.4597185475146262	T	T	T
15.9970898761711666	5.3274024896719538	8.9451241821253618	F	F	F
14.3973749958934487	2.6612077664659672	8.0000001838787966	F	F	F
15.9970904006310626	3.3057359944282361	8.9451248436730744	F	F	F
14.3973741099471670	0.6395412680809034	8.0000000000000000	F	F	F
14.3973775161791746	5.3274024165410783	11.7805090714841079	F	F	F
15.9970963262294603	2.6612076933350908	10.8353850732375427	F	F	F
14.3973780406390723	3.3057359212973605	11.7805097330318205	F	F	F
15.9970954402831786	0.6395411949500270	10.8353848893587461	F	F	F
15.9970724247237204	5.3275982192954334	14.6153449032076139	T	T	T
14.4099326216937662	2.6665708597312912	13.7001046244438900	T	T	T
15.9968748626528239	3.3343783974335928	14.7440543439455762	T	T	T
14.4044224200085829	0.6690646526973597	13.6536591894052179	T	T	T
14.4604402727224262	5.5138057319588789	17.5677386421210358	T	T	T
15.9966330575827822	2.7217999198717258	16.6673659995934891	T	T	T
14.3419428520595140	3.4539207351121735	17.6080065244298538	T	T	T
15.9972587378875932	0.7453398041171421	16.4456052786572577	T	T	T
0.0015052300591974	1.0709229231155921	19.6448223746435531	T	T	T
1.3410251349658873	2.3490840975396834	21.4523318105594676	T	T	T
0.0017774822369062	1.0555349564766501	23.2560200008619802	T	T	T
0.0034484722747468	3.7197272047504550	19.6065659155201466	T	T	T
1.3398507221246685	5.0361708873967261	21.3782286125828946	T	T	T
0.0063546146983217	3.7594784642362411	23.2636897060917676	T	T	T
2.7272704626339026	1.0977982667049890	19.6589149597478432	T	T	T
3.9993833591604271	2.4439040976828239	21.4669754278761857	T	T	T
2.7366648667821227	1.0815189165122403	23.2722300265256088	T	T	T
2.6169164541874199	3.7153544950524213	19.5636781935219339	T	T	T
3.9905672676267074	5.0331976476522291	21.3728620172961463	T	T	T
2.6401986508460737	3.7920416001368689	23.2786757411395762	T	T	T
5.3845732185887831	1.1416234837890098	19.6842598178308847	T	T	T
6.6582322368389555	2.5367998913104128	21.5133063536366436	T	T	T
5.4113304275055389	1.1197586572612801	23.2965634392469667	T	T	T
5.2959260381131612	3.7242888465103778	19.5470170283383489	T	T	T
6.6681381841003686	5.0690930410135682	21.3608974047987594	T	T	T
5.3055936207558156	3.8568560517108685	23.2896416290829400	T	T	T
8.0008772136147996	1.1698883915264544	19.6961579466702617	T	T	T
9.3435719201157035	2.5388623400951920	21.5085547716993624	T	T	T
8.0144699514191569	1.1398243570489901	23.2970744697724683	T	T	T
8.0010332520606617	3.7263407218234974	19.5506151057741491	T	T	T
9.3352154785553711	5.0665144616369959	21.3573940471869257	T	T	T

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  8.0021797713260394  3.8706980074054749 23.2945125757028748   T   T   T
 10.6204662861133041  1.1405480688162211 19.6852288636790149   T   T   T
 12.0033423449616130  2.4453764054163680 21.4668315989744833   T   T   T
 10.5926731956870164  1.1209506351366130 23.2970295667433867   T   T   T
 10.7111918041724561  3.7220246997513122 19.5453379476768561   T   T   T
 12.0128744707158202  5.0328981856502990 21.3744420444661074   T   T   T
 10.6952834209111440  3.8565930174436556 23.2883349877690833   T   T   T
 13.2739844397371662  1.0974270184874992 19.6595324799064279   T   T   T
 14.6620651875036785  2.3490530519280961 21.4514431505653533   T   T   T
 13.2700767327375893  1.0794161811138532 23.2726974758014222   T   T   T
 13.3867899039672622  3.7152583223048290 19.5639368691718936   T   T   T
 14.6620146419238804  5.0350303905963028 21.3785794920358612   T   T   T
 13.3630540770984645  3.7888740865436881 23.2794741771472751   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_6x2/Ru E_tot= -359.28813498 eV
 D3-zero damping= -13.1265247 eV, D3-BJ damping= -14.4764145 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
    15.9971684516400039    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3323894838800010    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.1312880290811052
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2
Selective dynamics
Cartesian
  3.1993551148591606  5.3274024896719538  8.9451241821253618   F   F   F
  1.5996402345814453  2.6612077664659672  8.0000001838787966   F   F   F
  3.1993556393190592  3.3057359944282361  8.9451248436730744   F   F   F
  1.5996393486351645  0.6395412680809034  8.0000000000000000   F   F   F
  1.5996427548671703  5.3274024165410783 11.7805090714841079   F   F   F
  3.1993615649174565  2.6612076933350908 10.8353850732375427   F   F   F
  1.5996432793270685  3.3057359212973605 11.7805097330318205   F   F   F
  3.1993606789711753  0.6395411949500270 10.8353848893587461   F   F   F
  3.1993467229492936  5.2718819364883602 14.5855789101692022   T   T   T
  1.5996569851816422  2.6466234728606866 13.6878147161161596   T   T   T
  3.1994387426826747  3.2860046627128843 14.6707221095070661   T   T   T
  1.5997035097621688  0.6426037950667890 13.6687320935685275   T   T   T
  1.5996106162511958  5.0595471598567299 17.1692065688480220   T   T   T
  3.1996164637260409  2.6024386194214202 16.6458444118821021   T   T   T
  1.5997141858004313  3.2347238532007552 17.5302634585025885   T   T   T
  3.1993811897421716  0.6123312198331449 16.5205419865311782   T   T   T
  6.3987888051871611  5.3274024896719538  8.9451241821253618   F   F   F
  4.7990739249094467  2.6612077664659672  8.0000001838787966   F   F   F
  6.3987893296470606  3.3057359944282361  8.9451248436730744   F   F   F
  4.7990730389631659  0.6395412680809034  8.0000000000000000   F   F   F
  4.7990764451951717  5.3274024165410783 11.7805090714841079   F   F   F
  6.3987952552454574  2.6612076933350908 10.8353850732375427   F   F   F
  4.7990769696550704  3.3057359212973605 11.7805097330318205   F   F   F
  6.3987943692991767  0.6395411949500270 10.8353848893587461   F   F   F
  6.3988597655728618  5.2720944592766266 14.5855337295177989   T   T   T
  4.7990279668653857  2.6465360468334680 13.6877584439650111   T   T   T
  6.3987560228453342  3.2860802743563799 14.6705633652550951   T   T   T
  4.7990759447594096  0.6424323499622524 13.6688108740024123   T   T   T
  4.7990565504811888  5.0597927147591761 17.1692821350049556   T   T   T
  6.3989256972835982  2.6024753643068994 16.6457977414127889   T   T   T
  4.7993760421491878  3.2348490779317829 17.5301642567675771   T   T   T
  6.3988887273514923  0.6122058286964474 16.5205443013573472   T   T   T
  9.5982224955151629  5.3274024896719538  8.9451241821253618   F   F   F
  7.9985076152374459  2.6612077664659672  8.0000001838787966   F   F   F
  9.5982230199750607  3.3057359944282361  8.9451248436730744   F   F   F
  7.9985067292911651  0.6395412680809034  8.0000000000000000   F   F   F
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  7.9985101355231736  5.3274024165410783 11.7805090714841079   F   F   F
  9.5982289455734584  2.6612076933350908 10.8353850732375427   F   F   F
  7.9985106599830704  3.3057359212973605 11.7805097330318205   F   F   F
  9.5982280596271767  0.6395411949500270 10.8353848893587461   F   F   F
  9.5982532066669464  5.2721313246064900 14.5855454776919942   T   T   T
  7.9985837231083980  2.6469013763699789 13.6878462481882401   T   T   T
  9.5983727426502501  3.2861038978720156 14.6705609227949303   T   T   T
  7.9985483903979944  0.6426436248741920 13.6687893471135986   T   T   T
  7.9985855628412637  5.0595684926042050 17.1695760728843076   T   T   T
  9.5981965523821771  2.6024942055000255 16.6457663768057671   T   T   T
  7.9985621930420434  3.2347714394153400 17.5301125036006624   T   T   T
  9.5982577123135258  0.6122071241872760 16.5205775422602628   T   T   T
 12.7976561858431630  5.3274024896719538  8.9451241821253618   F   F   F
 11.1979413055654486  2.6612077664659672  8.0000001838787966   F   F   F
 12.7976567103030643  3.3057359944282361  8.9451248436730744   F   F   F
 11.1979404196191688  0.6395412680809034  8.0000000000000000   F   F   F
 11.1979438258511745  5.3274024165410783 11.7805090714841079   F   F   F
 12.7976626359014620  2.6612076933350908 10.8353850732375427   F   F   F
 11.1979443503110723  3.3057359212973605 11.7805097330318205   F   F   F
 12.7976617499551804  0.6395411949500270 10.8353848893587461   F   F   F
 12.7977328517758639  5.2718874833962932 14.5855745145212463   T   T   T
 11.1981340013800512  2.6465788360950699 13.6877739905411850   T   T   T
 12.7977397787608353  3.2860131242064985 14.6707275601597900   T   T   T
 11.1980277373654555  0.6424626283374298 13.6688104378097819   T   T   T
 11.1981275176223818  5.0598139366799630 17.1692920887511669   T   T   T
 12.7975593647202555  2.6024507153182985 16.6458614023264175   T   T   T
 11.1977494672892561  3.2348611662595408 17.5301456250749652   T   T   T
 12.7977887970166027  0.6123411126827961 16.5205515094585671   T   T   T
 15.9970898761711666  5.3274024896719538  8.9451241821253618   F   F   F
 14.3973749958934487  2.6612077664659672  8.0000001838787966   F   F   F
 15.9970904006310626  3.3057359944282361  8.9451248436730744   F   F   F
 14.3973741099471670  0.6395412680809034  8.0000000000000000   F   F   F
 14.3973775161791746  5.3274024165410783 11.7805090714841079   F   F   F
 15.9970963262294603  2.6612076933350908 10.8353850732375427   F   F   F
 14.3973780406390723  3.3057359212973605 11.7805097330318205   F   F   F
 15.9970954402831786  0.6395411949500270 10.8353848893587461   F   F   F
 15.9971243949791244  5.2721354760478372 14.5854377341204344   T   T   T
 14.3975124094594680  2.6466175429719909 13.6878146549333728   T   T   T
 15.9971785734933380  3.2861877284695198 14.6706391174204676   T   T   T
 14.3974020272724026  0.6426073276043001 13.6687352911186899   T   T   T
 14.3975698013799214  5.0595509833683741 17.1691853968184738   T   T   T
 15.9971548116102156  2.6023523104315420 16.6457316728516460   T   T   T
 14.3974291764963631  3.2347226632212291 17.5302698572114046   T   T   T
 15.9971667400084314  0.6123601791974526 16.5204787823164345   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_6x2/Ru E_tot= -307.37764507 eV
 D3-zero damping= -11.3566606 eV, D3-BJ damping= -13.8525093 eV
Ru
 1.0000000000000000
    15.9971684516400039    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3323894838800010    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9359299014895974
  36
Cartesian
 -0.0003215868966237  0.0001387718232279  8.1410784579881561
  1.3323232493174966  1.3330636501915472  9.9739177255234246
 -0.0001410002600903  0.0001929913185468 11.8047325495218640
  0.0001706670415896  2.6660826274741467  8.1410838215256298
  1.3322781920166600  3.9993648917139777  9.9743275245493432
  0.0001337854851738  2.6660954481196524 11.8047388951360137
  2.6664669440643274 -0.0000727689688700  8.1417828597059536
  3.9994930548298928  1.3328991807497261  9.9704977617500514
  2.6675798699484656 -0.0000381639931106 11.8049495526376251
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  2.6664915358640044  2.6662178889634820  8.1418332397379451
  3.9991718274333867  3.9994977187633722  9.9705018466824260
  2.6677562951555469  2.6662026509677377 11.8048320234695776
  5.3321500084519879 -0.0000030739748064  8.1417959533235962
  6.6663094602395203  1.3330393898025503  9.9740659391442286
  5.3308404929501769 -0.0000005562718983 11.8049916632295293
  5.3322144117029282  2.6661292571565949  8.1418143678128931
  6.6662983633388997  3.9992573356383985  9.9741727406774068
  5.3308473193591404  2.6662093831486757 11.8049208846266858
  7.9987817055734221 -0.0001068851184878  8.1411351801380576
  9.3309045129500490  1.3331738534178306  9.9744237461764413
  7.9987773745987347 -0.0001723741224692 11.8047817913517115
  7.9983209800279900  2.6663149081286921  8.1411282494720574
  9.3309004880680924  3.9992591955637837  9.9739549228699040
  7.9983639241543978  2.6664147644873970 11.8047846515881574
 10.6650727993666532  0.0000421887315624  8.1417930372607152
 11.9978085755731971  1.3331458673329741  9.9704510148535270
 10.6663287318857058 -0.0000395765779863 11.8049345159039518
 10.6649584717015706  2.6661834810468141  8.1417674468029286
 11.9980304507959534  3.9992215683260937  9.9704804780410150
 10.6662063490507215  2.6661865533091405 11.8049639156164154
 13.3307863438701286  0.0000046022000189  8.1418013908218434
 14.6648556219071402  1.3331005115303276  9.9741737435426607
 13.3294326055911370 -0.0000083205320955 11.8049701046980093
 13.3307868123304925  2.6661842389202546  8.1417665942930579
 14.6648653907550024  3.9993138785631555  9.9740631993434796
 13.3294509642733559  2.6661786057093098 11.8049612048041652

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt3/Au E_tot= -299.26005252 eV
 D3-zero damping= -11.1295153 eV, D3-BJ damping= -13.0562424 eV
Al  O Al  O  H Au
 1.0000000000000000
     5.0207852410612288    0.0000000000000000    0.0000000000000000
    -2.5103926205306135    4.3481275657050009    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.8962793741743269
  11  18   1   3   3  12
Selective dynamics
Cartesian
  0.0247044121034588 -0.0625308022311505 12.3918657751636374   F   F   F
  2.5361687563263335  1.3891323315334845 16.7197825444342918   T   T   T
  0.0263427389135948 -0.0602501978513956 18.8695102363570726   T   T   T
  2.5373186437506137  1.3867877650577889 10.0985295441362872   F   F   F
  0.0246102381956744  2.8387879348814442 14.5561856244294283   F   F   F
  0.0597793630225213 -0.0478619084564347  9.7781175373791598   F   F   F
  2.5360631110131608  1.3899847131194389 14.0665571956713507   F   F   F
  0.0259225275721317  2.8385063953054521 18.2585672213125143   T   T   T
  0.0253241507902667 -0.0597918065905659 16.1687268564640938   T   T   T
  2.5374377626391280  1.3885573035370065 20.6104779605892041   T   T   T
  0.0305096901933443  2.8377436544732229 11.8834768182986359   F   F   F
  1.5838226982549284 -0.0582065988212350 11.0348070799988349   F   F   F
  4.0635604285369471  1.3925468357810777 15.3704718438465928   T   T   T
  1.5684588601650520  2.8359211556313508 19.6263564177198973   T   T   T
  0.7874507266268332  1.2638958224770560 17.4973053697096184   T   T   T
  3.3059457670674619  2.7827968908176342  8.8712015584813955   F   F   F
  0.7961666023037474  4.1710679342480956 13.2250185171475465   F   F   F
 -0.7545687608512360  1.2836096299404649 11.0371856277262950   F   F   F
  1.7692803175117209  2.7104553822680009 15.3698458936960645   T   T   T
 -0.7421284956523023  4.1746219291975519 19.6260031013116851   T   T   T
  3.5198355434042421 -0.0629397652951747 17.4966541372265993   T   T   T
  0.9799982986887555  1.3315208248663268  8.8494658732768272   F   F   F
 -1.5122546819135796  2.8405137803999083 13.2250148374957774   F   F   F
  1.7732843293228320  2.9456755686198335 11.0407582029264013   F   F   F
  1.7748299594409098  0.0656158335615444 15.3707513829922640   T   T   T
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 -0.7469944586281763  1.5037712369873570 19.6261720303860123   T   T   T
 -1.7184080323614830  2.9667406981887821 17.4967597967616655   T   T   T
  3.3774398069409406 -0.0003190838666069  8.9135372731794220   F   F   F
  0.7948518443039444  1.5038566426442745 13.2221143204608822   F   F   F
  0.0262376393193984  2.8371636705508529 20.8561785208791726   T   T   T
  3.4405561771276503  2.6532587899013858 21.7193967996201067   T   T   T
  0.9899472354629557  1.5381472414674733 21.7187186047730023   T   T   T
  3.1804224089652604 -0.0278638797336938 21.7198325464723254   T   T   T
  0.4389404827551274  2.2109947737804641  8.8276013437729759   F   F   F
  2.8001615377239291  2.6409139343999573  8.0391937587954807   F   F   F
  3.3114545670894286  0.3261129919503125  7.9999999999999991   F   F   F
 -0.8107442689878164  4.2646165973993782 26.0933747889061891   T   T   T
  0.0363428971200192  2.8207228296624809 28.4600521416915520   T   T   T
  3.3556731305518626  2.8332408888377247 23.7554917711979456   T   T   T
  1.7073989939477923  2.8276907999950658 26.0941533655638693   T   T   T
  2.5447194857995772  1.3698121956225395 28.4549954637974238   T   T   T
  3.3813311463472004  2.8189049372206521 30.8948430798795179   T   T   T
  0.8746110528942000  1.3787499211234338 30.8963692526866112   T   T   T
  5.8908403833981211  1.3520457440345401 23.7525396802814228   T   T   T
  1.7150009939945647  5.7133900557601356 26.0942564883557822   T   T   T
  2.5459780306398292  4.2697790824664148 28.4802237030698109   T   T   T
  0.8852331958526578  4.2894459989640579 23.7542248637224880   T   T   T
  0.8636781887966064  4.2740247872497239 30.8963672632590800   T   T   T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Au E_tot= -271.07690904 eV
 D3-zero damping= -4.1561829 eV, D3-BJ damping= -6.159886 eV
Al  O Al  O  H
 1.0000000000000000
     5.0207852410612288    0.0000000000000000    0.0000000000000000
    -2.5103926205306135    4.3481275657050018    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.6415426255987491
  11  18   1   3   6
Selective dynamics
Cartesian
  0.0247044121034588 -0.0625308022311505 12.3918657751636392   F   F   F
  2.5364137912308440  1.3868300826092428 16.7188266140611717   T   T   T
  0.0290850825327209 -0.0669576026223403 18.8423747583170176   T   T   T
  2.5373186437506132  1.3867877650577889 10.0985295441362890   F   F   F
  0.0246102381956744  2.8387879348814442 14.5561856244294301   F   F   F
  0.0597793630225213 -0.0478619084564347  9.7781175373791616   F   F   F
  2.5360631110131608  1.3899847131194389 14.0665571956713524   F   F   F
  0.0266905114092258  2.8368025782913540 18.2761024543838602   T   T   T
  0.0257339365434883 -0.0615177227263780 16.1615553591954324   T   T   T
  2.5483845621150514  1.3822171701915744 20.5524563001699008   T   T   T
  0.0305096901933443  2.8377436544732229 11.8834768182986377   F   F   F
  1.5838226982549282 -0.0582065988212350 11.0348070799988349   F   F   F
  4.0628336254873485  1.3913806868329717 15.3731529089540508   T   T   T
  1.5749805403853727  2.8338162998041980 19.6427642234109037   T   T   T
  0.7867164648475554  1.2602485021853393 17.5020591424315732   T   T   T
  3.3059457670674610  2.7827968908176342  8.8712015584813955   F   F   F
  0.7961666023037474  4.1710679342480956 13.2250185171475483   F   F   F
 -0.7545687608512360  1.2836096299404649 11.0371856277262967   F   F   F
  1.7685989489519534  2.7088865426633126 15.3730418677585927   T   T   T
 -0.7521460696806903  4.1572293131425297 19.6459030449005709   T   T   T
  3.5201697419864857 -0.0654865158680555 17.5025944923181633   T   T   T
  0.9799982986887554  1.3315208248663268  8.8494658732768272   F   F   F
 -1.5122546819135794  2.8405137803999088 13.2250148374957792   F   F   F
  1.7732843293228318  2.9456755686198335 11.0407582029264013   F   F   F
  1.7756992466882109  0.0653690337688362 15.3739079309177100   T   T   T
 -0.7425957560935259  1.4970508326251590 19.6460150803080857   T   T   T
 -1.7172356360859384  2.9633907877504324 17.4982296228542964   T   T   T
  3.3774398069409401 -0.0003190838666069  8.9135372731794220   F   F   F
  0.7948518443039443  1.5038566426442745 13.2221143204608840   F   F   F
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  0.0300119454631052  2.8237588754621088 20.8884995350696556   T   T   T
  3.4123950740098210  2.7193631060869676 21.7581004028491023   T   T   T
  1.0637914359999301  1.5571289676630271 21.7652933653577350   T   T   T
  3.1896249982994331 -0.0157811727560116 21.7630077084146087   T   T   T
  0.4389404827551273  2.2109947737804641  8.8276013437729759   F   F   F
  2.8001615377239286  2.6409139343999577  8.0391937587954807   F   F   F
  3.3114545670894282  0.3261129919503125  8.0000000000000000   F   F   F
  3.3700481143257508  2.3172796099661692 22.6417562805624435   T   T   T
  0.8035246405344917  0.7035994686530853 22.1457190018605061   T   T   T
  4.1495469310812680 -0.1589455298387449 21.8474658116656499   T   T   T

Oxidized reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Au E_tot= -252.23076343
eV
 D3-zero damping= -3.9115237 eV, D3-BJ damping= -5.8640786 eV
Al  O Al  O  H
 1.0000000000000000
     5.0207852410612288    0.0000000000000000    0.0000000000000000
    -2.5103926205306135    4.3481275657050018    0.0000000000000000
     0.0000000000000018    0.0000000000000032   29.8754197198952873
  11  18   1   3   3
Selective dynamics
Cartesian
  0.0247044121034588 -0.0625308022311505 12.3918657751636392   F   F   F
  2.5379674788063453  1.4113393893633461 16.7332272325247011   T   T   T
 -0.0697134181065097  0.0298904736578420 18.7583632463067822   T   T   T
  2.5373186437506132  1.3867877650577889 10.0985295441362890   F   F   F
  0.0246102381956744  2.8387879348814442 14.5561856244294301   F   F   F
  0.0597793630225213 -0.0478619084564347  9.7781175373791616   F   F   F
  2.5360631110131608  1.3899847131194389 14.0665571956713524   F   F   F
  0.0184985546268800  2.8343226091505196 18.3870824794720029   T   T   T
  0.0426489101665339 -0.0737105999327873 16.1257358746796449   T   T   T
  2.9482527827421139  1.8935812574658428 20.7467495071008408   T   T   T
  0.0305096901933443  2.8377436544732229 11.8834768182986377   F   F   F
  1.5838226982549282 -0.0582065988212350 11.0348070799988349   F   F   F
  4.0738991674998291  1.3954995577747440 15.3920268699466263   T   T   T
  1.5922787609949995  3.0440152190869214 19.7069148601643818   T   T   T
  0.8251786140127541  1.2861155863558762 17.5446572081398493   T   T   T
  3.3059457670674610  2.7827968908176342  8.8712015584813955   F   F   F
  0.7961666023037474  4.1710679342480956 13.2250185171475483   F   F   F
 -0.7545687608512360  1.2836096299404649 11.0371856277262967   F   F   F
  1.7712827383293557  2.7096813364073911 15.3659505875782845   T   T   T
 -0.8696640049688020  4.2165718095712243 19.7277917458036107   T   T   T
  3.4575814960446301 -0.0720390285775246 17.4947202746958688   T   T   T
  0.9799982986887554  1.3315208248663268  8.8494658732768272   F   F   F
 -1.5122546819135794  2.8405137803999088 13.2250148374957792   F   F   F
  1.7732843293228318  2.9456755686198335 11.0407582029264013   F   F   F
  1.7738350620406980  0.0772274930493580 15.3577922408223966   T   T   T
 -0.8203460340767620  1.5421709517608007 19.4402316383779521   T   T   T
 -1.7426988636681418  3.0277883480247820 17.4884030767050866   T   T   T
  3.3774398069409401 -0.0003190838666069  8.9135372731794220   F   F   F
  0.7948518443039443  1.5038566426442745 13.2221143204608840   F   F   F
  0.8318386244558784  3.4105029183437017 21.3995790677319704   T   T   T
  4.0247768600690428  3.4878101195651716 21.0351693212833304   T   T   T
  1.6459011213501922  2.0175352153359820 21.9902574720611419   T   T   T
  3.7510863215319570  0.7011016837948602 21.8066263863372178   T   T   T
  0.4389404827551273  2.2109947737804641  8.8276013437729759   F   F   F
  2.8001615377239286  2.6409139343999577  8.0391937587954807   F   F   F
  3.3114545670894282  0.3261129919503125  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Au E_tot= -42.63862553 eV
 D3-zero damping= -5.8784015 eV, D3-BJ damping= -5.9395813 eV
Au
 1.0000000000000000
```

```
     5.0207852410612288    0.0000000000000000    0.0000000000000000
     2.5103926205306144    4.3481275657049991    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.1884510584595631
  12
Cartesian
  5.8572745733696729  1.4489731533193795 10.4154035471762718
  5.8580695118352253  4.3481740138940355 10.4154008366834887
  5.0209994683246419  2.8985367092034440 15.1880813685493834
  2.5102449548892651  1.4495294813966610  8.0005703946064095
  3.3469029458735742  2.8992267377854590 10.4153823755358381
  1.6739143499707458  2.8991627297500533 12.7737862987038557
  2.5105896790493381  1.4491627390196555 15.1880503855233417
  5.0206404168980754  0.0001547458663685  8.0000000000000000
  2.5106252086037273  4.3478713868465828 15.1884510584595596
  4.1842835749623841  1.4488850053799252 12.7737940005022423
  5.0206393097978870  2.8989057635229751  8.0005704382453189
  4.1834916192185432  4.3480784790973770 12.7737862340784716

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ag E_tot= -293.11799631 eV
 D3-zero damping= -9.7044823 eV, D3-BJ damping= -12.7391354 eV
Al  O Al  O  H Ag
 1.0000000000000000
     4.9892192065539964    0.0000000000000000    0.0000000000000000
    -2.4946096032769973    4.3207905779250027    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.8882634248631689
  11  18   1   3   3  12
Selective dynamics
Cartesian
  0.0245490937045436 -0.0621376666226303 12.3918657751636392   F   F   F
  2.5290111435728586  1.3817319576696718 16.7205885475931773   T   T   T
  0.0448135215585790 -0.0571486464063035 18.8782464795969425   T   T   T
  2.5213663406707179  1.3780689315797077 10.0985295441362890   F   F   F
  0.0244555118748267  2.8209402728905801 14.5561856244294301   F   F   F
  0.0594035259083271 -0.0475609972281347  9.7781175373791616   F   F   F
  2.5201187015570339  1.3812457802011333 14.0665571956713524   F   F   F
  0.0378662973111134  2.8226539290078021 18.2703203704100865   T   T   T
  0.0305225084753653 -0.0596063686327990 16.1784344654937833   T   T   T
  2.5453648577132193  1.3854783236235395 20.6058333151418189   T   T   T
  0.0303178735974916  2.8199025579476826 11.8834768182986377   F   F   F
  1.5738650921144421 -0.0578406497876230 11.0348070799988349   F   F   F
  4.0430251344389365  1.3838597912809103 15.3749091819409589   T   T   T
  1.5837902070919527  2.8182929505055205 19.6453912966024475   T   T   T
  0.7935138319660390  1.2581907964171142 17.5074001045993946   T   T   T
  3.2851610505038358  2.7653012485097790  8.8712015584813955   F   F   F
  0.7911610461536273  4.1448441329853569 13.2250185171475483   F   F   F
 -0.7498247332938902  1.2755394847486041 11.0371856277262967   F   F   F
  1.7611106745203864  2.6950464458548034 15.3737286488584548   T   T   T
 -0.7179172768350509  4.1570421043502543 19.6431222699492061   T   T   T
  3.5072901951933280 -0.0615014331287815 17.5062025642342505   T   T   T
  0.9738369795667092  1.3231494585786217  8.8494658732768272   F   F   F
 -1.5027470289905642  2.8226552678953150 13.2250148374957792   F   F   F
  1.7621355644099737  2.9271558964606417 11.0407582029264013   F   F   F
  1.7665667840232842  0.0639898324316678 15.3744012369539433   T   T   T
 -0.7254802259975335  1.4965815418070894 19.6443176760656435   T   T   T
 -1.6961130892405103  2.9486794027352907 17.5068048815574642   T   T   T
  3.3562056022551681 -0.0003170777636050  8.9135372731794220   F   F   F
  0.7898545541310364  1.4944017887924486 13.2221143204608840   F   F   F
  0.0517248583043726  2.8277478685084825 20.8615962765503582   T   T   T
  3.4409534595621758  2.6570735672384549 21.7758679533891275   T   T   T
  1.0022900525342755  1.5297358935250489 21.7828057811108771   T   T   T
  3.2008821974209782 -0.0199476146024889 21.7727121030107185   T   T   T
  0.4361808326685323  2.1970940921194195  8.8276013437729759   F   F   F
  2.7825567226438599  2.6243103203472926  8.0391937587954807   F   F   F
```

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  3.2906352163076003  0.3240626963365961  8.0000000000000000   F   F   F
  0.0992084987403692  2.8621324943927822 25.7030377946139446   T   T   T
  0.9415317965746410  1.4313255384492625 28.0645678850217593   T   T   T
  4.2492696243195835  1.3480774640698383 23.4184057353588386   T   T   T
  2.5919488723929995  1.4239121570471382 25.7225958612086814   T   T   T
  3.4316885785744975 -0.0129799011909652 28.0650131151628095   T   T   T
  4.2795420927840473  1.4343115267333388 30.4393605959645797   T   T   T
  1.7862822739960631 -0.0064132001003087 30.4396700498728485   T   T   T
  6.6788628579957612 -0.0149428883715071 23.4248241296028397   T   T   T
  2.5906708014894098  4.3022564209249836 25.7495034685891966   T   T   T
  3.4398278570197589  2.8660074567596747 28.0636782135082434   T   T   T
  1.7886805765113802  2.8906043023550088 23.4091894198235906   T   T   T
  1.7859688161059417  2.8721568165114690 30.4361583626124705   T   T   T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ag E_tot= -271.55246169 eV
 D3-zero damping= -4.2127902 eV, D3-BJ damping= -6.2322991 eV
Al  O Al  O  H
 1.0000000000000000
     4.9892192065539955    0.0000000000000000    0.0000000000000000
    -2.4946096032769969    4.3207905779250009    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.6586255281375628
  11  18   1   3   6
Selective dynamics
Cartesian
  0.0245490937045436 -0.0621376666226303 12.3918657751636392   F   F   F
  2.5195384007609727  1.3779860146239264 16.7212522149315745   T   T   T
  0.0283123171433804 -0.0666928050656738 18.8515086544505124   T   T   T
  2.5213663406707174  1.3780689315797072 10.0985295441362890   F   F   F
  0.0244555118748270  2.8209402728905792 14.5561856244294301   F   F   F
  0.0594035259083271 -0.0475609972281347  9.7781175373791616   F   F   F
  2.5201187015570334  1.3812457802011331 14.0665571956713524   F   F   F
  0.0260100715758213  2.8190148612444306 18.2939674626710733   T   T   T
  0.0250808918051636 -0.0609256055309718 16.1715327600455865   T   T   T
  2.5323285567372364  1.3730830082670051 20.5701512275968952   T   T   T
  0.0303178735974918  2.8199025579476822 11.8834768182986377   F   F   F
  1.5738650921144419 -0.0578406497876229 11.0348070799988349   F   F   F
  4.0388039415577150  1.3824005851982362 15.3769377440422836   T   T   T
  1.5664576871684674  2.8140961102768109 19.6578829953023906   T   T   T
  0.7818161141924985  1.2537225090826760 17.5118549393748140   T   T   T
  3.2851610505038358  2.7653012485097781  8.8712015584813955   F   F   F
  0.7911610461536276  4.1448441329853560 13.2250185171475483   F   F   F
 -0.7498247332938900  1.2755394847486039 11.0371856277262967   F   F   F
  1.7567044911700047  2.6935928520696644 15.3769299014876655   T   T   T
 -0.7470031566915653  4.1336072177059169 19.6615119408494046   T   T   T
  3.4956760426325109 -0.0646725121165227 17.5127706014026678   T   T   T
  0.9738369795667091  1.3231494585786212  8.8494658732768272   F   F   F
 -1.5027470289905638  2.8226552678953145 13.2250148374957792   F   F   F
  1.7621355644099737  2.9271558964606408 11.0407582029264013   F   F   F
  1.7631305609493964  0.0634822623535510 15.3777675341989362   T   T   T
 -0.7396324422515000  1.4877676801839985 19.6617455572628508   T   T   T
 -1.7065676593537358  2.9437488484435930 17.5083212268248332   T   T   T
  3.3562056022551676 -0.0003170777636050  8.9135372731794220   F   F   F
  0.7898545541310364  1.4944017887924481 13.2221143204608840   F   F   F
  0.0299095760234140  2.8060049471902464 20.9069805028898514   T   T   T
  3.3839225085352598  2.7162746435163374 21.7796694245989677   T   T   T
  1.0532708817409016  1.5389103378071014 21.7879041602799255   T   T   T
  3.1814001659501479 -0.0146856574922347 21.7835754333733860   T   T   T
  0.4361808326685325  2.1970940921194186  8.8276013437729759   F   F   F
  2.7825567226438603  2.6243103203472917  8.0391937587954807   F   F   F
  3.2906352163075998  0.3240626963365960  8.0000000000000000   F   F   F
  3.3446914313372353  2.3035949527237101 22.6588380742533175   T   T   T
  0.7968980527097930  0.6794617823488395 22.1579637643251175   T   T   T
  4.1408247048957278 -0.1682656992762342 21.8592225970674185   T   T   T
```

```
Oxidized reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ag E_tot= -252.64261481
eV
 D3-zero damping= -3.9637164 eV, D3-BJ damping= -5.9319414 eV
Al  O Al  O  H
 1.0000000000000000
     4.9892192065539955    0.0000000000000000    0.0000000000000000
    -2.4946096032769969    4.3207905779250009    0.0000000000000000
     0.0000000000000018    0.0000000000000032   29.8754197198952873
  11  18   1   3   3
Selective dynamics
Cartesian
  0.0245490937045436 -0.0621376666226303 12.3918657751636392   F   F   F
  2.5229213449934109  1.3993245493572584 16.7362940475435380   T   T   T
 -0.0687007946142963  0.0236050345472931 18.7724096843552672   T   T   T
  2.5213663406707174  1.3780689315797072 10.0985295441362890   F   F   F
  0.0244555118748270  2.8209402728905792 14.5561856244294301   F   F   F
  0.0594035259083271 -0.0475609972281347  9.7781175373791616   F   F   F
  2.5201187015570334  1.3812457802011331 14.0665571956713524   F   F   F
  0.0185940800719443  2.8134773580990635 18.4046034663818787   T   T   T
  0.0416995292790613 -0.0729293296689340 16.1404468156682697   T   T   T
  2.9133434233809883  1.8662452133992922 20.7542050573082832   T   T   T
  0.0303178735974918  2.8199025579476822 11.8834768182986377   F   F   F
  1.5738650921144419 -0.0578406497876229 11.0348070799988349   F   F   F
  4.0496112483166371  1.3858414711158229 15.3977025731562520   T   T   T
  1.5790150886828462  3.0152769224581779 19.7286173261357369   T   T   T
  0.8200994421694132  1.2761631024636892 17.5547001156877620   T   T   T
  3.2851610505038358  2.7653012485097781  8.8712015584813955   F   F   F
  0.7911610461536276  4.1448441329853560 13.2250185171475483   F   F   F
 -0.7498247332938900  1.2755394847486039 11.0371856277262967   F   F   F
  1.7600337029591737  2.6934304896622598 15.3717312413844418   T   T   T
 -0.8633786145810906  4.2023174082000132 19.7555818255111291   T   T   T
  3.4355792910914231 -0.0761530885446821 17.5068997202889243   T   T   T
  0.9738369795667091  1.3231494585786212  8.8494658732768272   F   F   F
 -1.5027470289905638  2.8226552678953145 13.2250148374957792   F   F   F
  1.7621355644099737  2.9271558964606408 11.0407582029264013   F   F   F
  1.7621775509196023  0.0737802926749482 15.3636538771481757   T   T   T
 -0.8197770395167491  1.5286575687441712 19.4561682645953056   T   T   T
 -1.7292655477191268  3.0045043145924257 17.5038688794896942   T   T   T
  3.3562056022551676 -0.0003170777636050  8.9135372731794220   F   F   F
  0.7898545541310364  1.4944017887924481 13.2221143204608840   F   F   F
  0.8198832111249035  3.3796753565641593 21.4295103591688729   T   T   T
  3.9858537530646583  3.4662949724890515 21.0575561103477646   T   T   T
  1.6224137099169911  1.9794761684756597 22.0175247868710358   T   T   T
  3.7323408232614770  0.6976754929876240 21.8323098539947829   T   T   T
  0.4361808326685325  2.1970940921194186  8.8276013437729759   F   F   F
  2.7825567226438603  2.6243103203472917  8.0391937587954807   F   F   F
  3.2906352163075998  0.3240626963365960  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ag E_tot= -34.93293542 eV
 D3-zero damping= -4.3721298 eV, D3-BJ damping= -5.4169809 eV
Ag
 1.0000000000000000
     4.9892192065539964    0.0000000000000000    0.0000000000000000
     2.4946096032769982    4.3207905779250000    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.0795847403917733
  12
Cartesian
  5.8207103770049606  1.4402884322230407 10.3699668397062723
  5.8207421296715482  4.3208250380505557 10.3699653615784406
  4.9893354737130222  2.8803918737569485 15.0795263970611622
  2.4945236448711592  1.4403588282938187  8.0000560297603656
  3.3261123009183318  2.8805715803445779 10.3699658515051176
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  1.6631335541781627  2.8804617680119411 12.7102937657415538
  2.4947289682325886  1.4401316754582061 15.0795252626000682
  4.9891266505965275  0.0001020320955719  8.0000000000000000
  2.4947677325361566  4.3206221229474151 15.0795847403917733
  4.1577404951933525  1.4402001477997917 12.7102863423017887
  4.9891330678717347  2.8806229254474403  8.0000595444143716
  4.1577428402490870  4.3207255949594137 12.7102958358489708

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt3/Cu E_tot= -295.37630409 eV
 D3-zero damping= -10.6453788 eV, D3-BJ damping= -14.1914953 eV
Al  O Al  O  H Cu
 1.0000000000000000
     4.3712972374160088    0.0000000000000000    0.0000000000000000
    -2.1856486187080035    3.7856544550950009    0.0000000000000000
     0.0000000000000023    0.0000000000000041   38.3178570262291203
  11  18   1   3   3  12
Selective dynamics
Cartesian
  0.0215086531677685 -0.0544418273084030 12.3918657751636410   F   F   F
  2.2078884272457353  1.2091154814373477 16.7681008793878377   T   T   T
  0.0224679763328455 -0.0535983250363465 19.0641482259051145   T   T   T
  2.2090914957212631  1.2073931138703942 10.0985295441362908   F   F   F
  0.0214266615821562  2.4715627658940180 14.5561856244294319   F   F   F
  0.0520463138510189 -0.0416704993677141  9.7781175373791633   F   F   F
  2.2079983785048909  1.2101765052243529 14.0665571956713542   F   F   F
  0.0225438697138202  2.4703127064442874 18.6807096976686857   T   T   T
  0.0222273025146587 -0.0525094026500669 16.4232528182621209   T   T   T
  2.2081448196992302  1.2085575702241009 21.0498165200674094   T   T   T
  0.0265629613801997  2.4706535734381823 11.8834768182986394   F   F   F
  1.3789396385285673 -0.0506770021839981 11.0348070799988367   F   F   F
  3.5697365212253258  1.1976840339968016 15.4590862208553634   T   T   T
  1.3991859240550866  2.4540672820484728 20.0094093216895672   T   T   T
  0.7074632369573549  1.1305452391965869 17.7347100552075609   T   T   T
  2.8782891330310356  2.4228147146460746  8.8712015584813972   F   F   F
  0.6931746135466345  3.6314992302278499 13.2250185171475501   F   F   F
 -0.6569578624422990  1.1175620863825977 11.0371856277262985   F   F   F
  1.5367529280735834  2.3942967329322746 15.4588579570212481   T   T   T
 -0.6515923810804081  3.6710097270942486 20.0094279137676381   T   T   T
  3.0260788617570120 -0.0518460075198281 17.7346690549481920   T   T   T
  0.8532258700683000  1.1592754965296630  8.8494658732768290   F   F   F
 -1.3166296497320427  2.4730653563026599 13.2250148374957810   F   F   F
  1.5438925422517320  2.5646234318339527 11.0407582029264031   F   F   F
  1.5169595637226330  0.0359803302491310 15.4594534160865376   T   T   T
 -0.6797918392968447  1.2865318708059679 20.0094826521796136   T   T   T
 -1.4805637466981563  2.5474141639480048 17.7348019842460758   T   T   T
  2.9405347149441532 -0.0002778072268846  8.9135372731794238   F   F   F
  0.6920299324387056  1.3093179795260763 13.2221143204608858   F   F   F
  0.0222325682018336  2.4707182792556859 21.2789353809983730   T   T   T
  2.8887075316752058  2.4607283243790525 22.2673617276411768   T   T   T
  0.7838346154122494  1.1731145962397627 22.2677853268766981   T   T   T
  2.9517385047024924 -0.0063561214242826 22.2673545564009316   T   T   T
  0.3821592096721468  1.9249808311906467  8.8276013437729777   F   F   F
  2.4379330735094276  2.2992857155658606  8.0391937587954825   F   F   F
  2.8830853155326417  0.2839270656588687  8.0000000000000018   F   F   F
 -0.7036416778638754  3.7246887735029985 26.1767335915674444   T   T   T
  0.0260520571352913  2.4628909174676661 28.2433460274502757   T   T   T
  2.9326623821031887  2.4656094077976212 24.1309590002826724   T   T   T
  1.4799454599393778  2.4647977152686531 26.1768029553258508   T   T   T
  2.2117077755737182  1.2009900675696732 28.2413248918344415   T   T   T
  2.9396622045833869  2.4624354613066046 30.3180470300429086   T   T   T
  0.7545339969708696  1.2013244950802895 30.3180347303789084   T   T   T
  5.1259275744366350  1.1958132020791079 24.1313428754129475   T   T   T
  1.4825972129269402  4.9894504596283289 26.1768103198645079   T   T   T
```

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  2.2117211155670335  3.7247754541128990 28.2423260378988559   T   T   T
  0.7578323126840205  3.7302417501839198 24.1309327573444889   T   T   T
  0.7536239884854736  3.7251335695747509 30.3179689762250355   T   T   T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Cu E_tot= -261.80319715 eV
 D3-zero damping= -5.3491477 eV, D3-BJ damping= -7.9298342 eV
Al  O Al  O  H
 1.0000000000000000
     4.3712972374160088    0.0000000000000000    0.0000000000000000
    -2.1856486187080040    3.7856544550950013    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.0727044460749156
  11  18   1   3   6
Selective dynamics
Cartesian
  0.0215086531677685 -0.0544418273084030 12.3918657751636392   F   F   F
  2.2060661634981908  1.2128086092904191 16.7694536498040456   T   T   T
  0.0197772019037295 -0.0474852411907535 19.0585841459243248   T   T   T
  2.2090914957212626  1.2073931138703942 10.0985295441362890   F   F   F
  0.0214266615821559  2.4715627658940180 14.5561856244294301   F   F   F
  0.0520463138510189 -0.0416704993677141  9.7781175373791616   F   F   F
  2.2079983785048904  1.2101765052243532 14.0665571956713524   F   F   F
  0.0196522258582338  2.4769201030025751 18.6893928466874151   T   T   T
  0.0210594271086068 -0.0496967564970262 16.4236249100486340   T   T   T
  2.2140025851318805  1.2070014985951170 21.0217298554385188   T   T   T
  0.0265629613801994  2.4706535734381823 11.8834768182986377   F   F   F
  1.3789396385285673 -0.0506770021839981 11.0348070799988349   F   F   F
  3.5683995929545973  1.1997532561303290 15.4603111312232127   T   T   T
  1.4007969570591159  2.4652699118338912 20.0163356644795272   T   T   T
  0.7059778523563874  1.1371039418188500 17.7386183468378711   T   T   T
  2.8782891330310352  2.4228147146460746  8.8712015584813955   F   F   F
  0.6931746135466340  3.6314992302278499 13.2250185171475483   F   F   F
 -0.6569578624422991  1.1175620863825979 11.0371856277262967   F   F   F
  1.5355749582901901  2.3966121239713365 15.4602199494527550   T   T   T
 -0.6687346188136337  3.6636940971954712 20.0241743890855446   T   T   T
  3.0223970426333864 -0.0462402963761508 17.7401801393031135   T   T   T
  0.8532258700682998  1.1592754965296632  8.8494658732768272   F   F   F
 -1.3166296497320427  2.4730653563026603 13.2250148374957792   F   F   F
  1.5438925422517316  2.5646234318339531 11.0407582029264013   F   F   F
  1.5164661360793703  0.0376134046236786 15.4601464443399745   T   T   T
 -0.6758279306224818  1.2936533472902760 20.0093422849179632   T   T   T
 -1.4817071268832356  2.5524292498360990 17.7357028655543658   T   T   T
  2.9405347149441527 -0.0002778072268846  8.9135372731794220   F   F   F
  0.6920299324387055  1.3093179795260765 13.2221143204608840   F   F   F
  0.0260587330530712  2.4631689461449700 21.2980366348874703   T   T   T
  2.9032488308801598  2.5199576097471716 22.3088648659639759   T   T   T
  0.8578590474134370  1.2838140162492633 22.3063269794706720   T   T   T
  2.8975374185732972  0.0253744326717403 22.2695249801704129   T   T   T
  0.3821592096721466  1.9249808311906469  8.8276013437729759   F   F   F
  2.4379330735094271  2.2992857155658606  8.0391937587954807   F   F   F
  2.8830853155326417  0.2839270656588688  8.0000000000000000   F   F   F
  2.9312916432652747  1.9162183597666755 23.0728130116087229   T   T   T
  0.7808217239076614  0.3653194789588693 22.6200786269831156   T   T   T
  3.8122260134129511 -0.3249153011256679 22.3480177168884282   T   T   T

Oxidized reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Cu E_tot= -244.13833363
eV
 D3-zero damping= -5.0614669 eV, D3-BJ damping= -7.5940439 eV
Al  O Al  O  H
 1.0000000000000000
     4.3712972374160088    0.0000000000000000    0.0000000000000000
    -2.1856486187080040    3.7856544550950013    0.0000000000000000
     0.0000000000000018    0.0000000000000032   29.8754197198952873
  11  18   1   3   3
```

```
Selective dynamics
Cartesian
  0.0215086531677685 -0.0544418273084030 12.3918657751636392   F   F   F
  2.2081615258939840  1.2088342260985048 16.7679369666259888   T   T   T
  0.0208494501510796 -0.0571010772495825 19.0504502554157966   T   T   T
  2.2090914957212626  1.2073931138703942 10.0985295441362890   F   F   F
  0.0214266615821559  2.4715627658940180 14.5561856244294301   F   F   F
  0.0520463138510189 -0.0416704993677141  9.7781175373791616   F   F   F
  2.2079983785048904  1.2101765052243532 14.0665571956713524   F   F   F
  0.0323592980175018  2.4718698901986165 18.7037541097228797   T   T   T
  0.0237422479616174 -0.0536033841123026 16.4237169911173275   T   T   T
  2.2139322324373696  1.1875188261051066 20.9221359434802601   T   T   T
  0.0265629613801994  2.4706535734381823 11.8834768182986377   F   F   F
  1.3789396385285673 -0.0506770021839981 11.0348070799988349   F   F   F
  3.5705737814677940  1.1964544016036949 15.4612449856843739   T   T   T
  1.3918558783898827  2.4691335164517518 20.0014242795803092   T   T   T
  0.7045020847340002  1.1329546335488077 17.7390051569164982   T   T   T
  2.8782891330310352  2.4228147146460746  8.8712015584813955   F   F   F
  0.6931746135466340  3.6314992302278499 13.2250185171475483   F   F   F
 -0.6569578624422991  1.1175620863825979 11.0371856277262967   F   F   F
  1.5357389267651276  2.3933604518992029 15.4656419428122369   T   T   T
 -0.6659532296868176  3.6490131846780787 19.9764615962844019   T   T   T
  3.0279444299339953 -0.0451088831117361 17.7468676780492132   T   T   T
  0.8532258700682998  1.1592754965296632  8.8494658732768272   F   F   F
 -1.3166296497320427  2.4730653563026603 13.2250148374957792   F   F   F
  1.5438925422517316  2.5646234318339531 11.0407582029264013   F   F   F
  1.5193742881339378  0.0338879291998426 15.4670402621589513   T   T   T
 -0.6021098029606526  1.2688198096357135 20.1102023380287989   T   T   T
 -1.4737124294508699  2.5368781658424160 17.7446536018163776   T   T   T
  2.9405347149441527 -0.0002778072268846  8.9135372731794220   F   F   F
  0.6920299324387055  1.3093179795260765 13.2221143204608840   F   F   F
 -0.0378337837647317  2.5006652406707368 21.4155302260902296   T   T   T
  2.6919931707394285  2.6133549289782225 22.3534321866651098   T   T   T
  1.4406790682010437  1.8568509122031169 22.5256006130744666   T   T   T
  2.5767064895737155  0.1176422962678369 22.3458748120086170   T   T   T
  0.3821592096721466  1.9249808311906469  8.8276013437729759   F   F   F
  2.4379330735094271  2.2992857155658606  8.0391937587954807   F   F   F
  2.8830853155326417  0.2839270656588688  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Cu E_tot= -46.32239467 eV
 D3-zero damping= -4.3621417 eV, D3-BJ damping= -5.3255084 eV
Cu
 1.0000000000000000
     4.3712972374160088    0.0000000000000000    0.0000000000000000
     2.1856486187080044    3.7856544550949991    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.1910562705090015
  12
Cartesian
  5.0998395037423112  1.2618881788428995 10.0692388600749183
  5.0998394815583401  3.7856577222838950 10.0692388369305323
  4.3713715760769913  2.5236955363934421 14.1910562705089980
  2.1856126228030477  1.2619174447456631  8.0000000599177330
  2.9141908829507575  2.5237729685808548 10.0692388040251863
  1.4571309268965353  2.5237401457261202 12.1219743229249115
  2.1857229184353835  1.2618107213504677 14.1910561280621899
  4.3712611973561959  0.0000326417149119  8.0000001557311613
  2.1857229844484767  3.7855804354035851 14.1910561453164430
  3.6427795892181440  1.2618553396925982 12.1219742618574671
  4.3712612470000343  2.5238022950423686  8.0000000000000000
  3.6427796691557450  3.7856249270563578 12.1219742822319443

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt3/Pt E_tot= -336.77703434 eV
 D3-zero damping= -12.472116 eV, D3-BJ damping= -14.7519881 eV
```

```
Al  O Al  O  H Pt
 1.0000000000000000
     4.7985659889076251    0.0000000000000000    0.0000000000000000
    -2.3992829944538117    4.1556800481300007    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.6601680551931963
  11  18   1   3   3  12
Selective dynamics
Cartesian
  0.0236109982809300 -0.0597631976750483 12.3918657751636392   F   F   F
  2.4247946512784697  1.3256883738101966 16.7360119571121793   T   T   T
  0.0278010225764368 -0.0616289672844198 18.9315107147496242   T   T   T
  2.4250172756541604  1.3254087326453665 10.0985295441362890   F   F   F
  0.0235209924971256  2.7131435781475779 14.5561856244294301   F   F   F
  0.0571335367807529 -0.0457435470860158  9.7781175373791616   F   F   F
  2.4238173126199665  1.3284641842331932 14.0665571956713524   F   F   F
  0.0266162972253694  2.7100058052655518 18.3870460399025042   T   T   T
  0.0249617371409416 -0.0588654076397197 16.2461288257563652   T   T   T
  2.4278343628769390  1.3223392044199120 20.7193324434834416   T   T   T
  0.0291593355749563  2.7121455174440863 11.8834768182986377   F   F   F
  1.5137229272725468 -0.0556303829029206 11.0348070799988349   F   F   F
  3.8956929057033260  1.3279012523967715 15.4035009017811806   T   T   T
  1.5108503498674917  2.6914431389364615 19.7517876431560211   T   T   T
  0.7605120054141491  1.2117519420181928 17.5776216850240594   T   T   T
  3.1596250700557684  2.6596306898585667  8.8712015584813955   F   F   F
  0.7609283799024609  3.9864570511834034 13.2250185171475483   F   F   F
 -0.7211716530913767  1.2267972473494415 11.0371856277262967   F   F   F
  1.6874454630380051  2.6007407800040903 15.4028526663820280   T   T   T
 -0.6985084093022472  4.0006665348149903 19.7519350285443629   T   T   T
  3.3560336661779115 -0.0603438467515591 17.5770002987499012   T   T   T
  0.9366237111311351  1.2725878994926449  8.8494658732768272   F   F   F
 -1.4453225013191369  2.7147930379849123 13.2250148374957792   F   F   F
  1.6947990130629129  2.8153003801747123 11.0407582029264013   F   F   F
  1.6889814125125751  0.0530857782475282 15.4035952239995151   T   T   T
 -0.7283477480440077  1.4329988165144678 19.7516561928940355   T   T   T
 -1.6387409847295371  2.8240941459778877 17.5771432545497177   T   T   T
  3.2279547937294235 -0.0003049612593239  8.9135372731794220   F   F   F
  0.7596718129077398  1.4372961580926580 13.2221143204608840   F   F   F
  0.0286273099197161  2.7068252959740837 20.9795836552996384   T   T   T
  3.2401922140682511  2.6131305362972364 21.8845429300908272   T   T   T
  0.9037132815944621  1.3773648668116869 21.8831543952301288   T   T   T
  3.1423806399831906 -0.0283785891970987 21.8839757519741944   T   T   T
  0.4195130384143357  2.1131364545026670  8.8276013437729759   F   F   F
  2.6762267799228221  2.5240274532366351  8.0391937587954807   F   F   F
  3.1648900513596718  0.3116792765633036  8.0000000000000000   F   F   F
 -0.7662903637994952  4.0760048331931111 26.0837932598885516   T   T   T
  0.0413764822201086  2.6905713996518656 28.3484161333688505   T   T   T
  3.2325879435781664  2.6875310546692139 23.8371783976960927   T   T   T
  1.6359677569517230  2.6976776698476521 26.0840957069117927   T   T   T
  2.4408505735903607  1.3051285498607756 28.3442018021070048   T   T   T
  3.2425547704268767  2.6879744177525877 30.6633109630360998   T   T   T
  0.8441556676880364  1.2935870658031867 30.6625083038970452   T   T   T
  5.6425575375604060  1.3176600961617526 23.8356151569008041   T   T   T
  1.6407348253401479  5.4618574435890572 26.0845753025225484   T   T   T
  2.4411855545188659  4.0750250813158990 28.3329176560008911   T   T   T
  0.8259457099565699  4.0903031690867095 23.8360616338946762   T   T   T
  0.8509466272840072  4.0697684386800015 30.6632760261094255   T   T   T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Pt E_tot= -272.60507144 eV
 D3-zero damping= -4.5616026 eV, D3-BJ damping= -6.6948757 eV
Al  O Al  O  H
 1.0000000000000000
     4.7985659889076251    0.0000000000000000    0.0000000000000000
    -2.3992829944538117    4.1556800481300007    0.0000000000000000
```

```
     0.0000000000000019    0.0000000000000033   30.7788761145800756
  11  18   1   3   6
Selective dynamics
Cartesian
  0.0236109982809300 -0.0597631976750483 12.3918657751636392   F   F   F
  2.4231143923534564  1.3281898190357051 16.7359412218488934   T   T   T
  0.0246836367654409 -0.0592074405223228 18.9131711386600756   T   T   T
  2.4250172756541604  1.3254087326453665 10.0985295441362890   F   F   F
  0.0235209924971256  2.7131435781475779 14.5561856244294301   F   F   F
  0.0571335367807529 -0.0457435470860158  9.7781175373791616   F   F   F
  2.4238173126199665  1.3284641842331932 14.0665571956713524   F   F   F
  0.0244069160029907  2.7143502608832777 18.4080373415487735   T   T   T
  0.0243746871235879 -0.0569226840627053 16.2413585407334580   T   T   T
  2.4325371936993871  1.3215495174646559 20.6919243111447670   T   T   T
  0.0291593355749563  2.7121455174440863 11.8834768182986377   F   F   F
  1.5137229272725468 -0.0556303829029206 11.0348070799988349   F   F   F
  3.8943416222109586  1.3284330892160623 15.4013660248776318   T   T   T
  1.5123701868957142  2.7034672361502921 19.7576439865202893   T   T   T
  0.7572842276310570  1.2169739246784856 17.5780037723388993   T   T   T
  3.1596250700557684  2.6596306898585667  8.8712015584813955   F   F   F
  0.7609283799024609  3.9864570511834034 13.2250185171475483   F   F   F
 -0.7211716530913767  1.2267972473494415 11.0371856277262967   F   F   F
  1.6869716341113155  2.6019879847598082 15.4011887006387802   T   T   T
 -0.7194890561724694  3.9911323128164398 19.7636288896313133   T   T   T
  3.3519284954802053 -0.0579023236949753 17.5788236888571276   T   T   T
  0.9366237111311351  1.2725878994926449  8.8494658732768272   F   F   F
 -1.4453225013191369  2.7147930379849123 13.2250148374957792   F   F   F
  1.6947990130629129  2.8153003801747123 11.0407582029264013   F   F   F
  1.6885165929725783  0.0548551381708277 15.4015223182526384   T   T   T
 -0.7221020307253820  1.4327031535589150 19.7636283666592902   T   T   T
 -1.6375311740624852  2.8256656195689756 17.5746534478961749   T   T   T
  3.2279547937294235 -0.0003049612593239  8.9135372731794220   F   F   F
  0.7596718129077398  1.4372961580926580 13.2221143204608840   F   F   F
  0.0276815721400276  2.7010084018863840 21.0260367394144900   T   T   T
  3.2136585375303879  2.6926540468477800 21.9213063682913223   T   T   T
  0.9889626434301658  1.4416324547594921 21.9355855680431659   T   T   T
  3.1137588045267233 -0.0023442938644196 21.9202622180212572   T   T   T
  0.4195130384143357  2.1131364545026670  8.8276013437729759   F   F   F
  2.6762267799228221  2.5240274532366351  8.0391937587954807   F   F   F
  3.1648900513596718  0.3116792765633036  8.0000000000000000   F   F   F
  3.1848091656500510  2.2336301167345263 22.7787529631674701   T   T   T
  0.7667558506982667  0.5465092207069606 22.2432015629774753   T   T   T
  4.0651205558462440 -0.2199230048511535 21.9633795830668070   T   T   T

Oxidized reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Pt E_tot= -252.89728248
eV
 D3-zero damping= -4.2814753 eV, D3-BJ damping= -6.3916524 eV
Al  O Al  O  H
 1.0000000000000000
     4.7985659889076251    0.0000000000000000    0.0000000000000000
    -2.3992829944538117    4.1556800481300007    0.0000000000000000
     0.0000000000000018    0.0000000000000032   29.8754197198952873
  11  18   1   3   3
Selective dynamics
Cartesian
  0.0236109982809300 -0.0597631976750483 12.3918657751636392   F   F   F
  2.4240061405460738  1.3266469974048365 16.7349490533366669   T   T   T
  0.0247239853232397 -0.0577304921763878 18.9139480052328111   T   T   T
  2.4250172756541604  1.3254087326453665 10.0985295441362890   F   F   F
  0.0235209924971256  2.7131435781475779 14.5561856244294301   F   F   F
  0.0571335367807529 -0.0457435470860158  9.7781175373791616   F   F   F
  2.4238173126199665  1.3284641842331932 14.0665571956713524   F   F   F
  0.0243385445352340  2.7123656405628691 18.4128495248146216   T   T   T
```

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  0.0242744393200570 -0.0580522588849449 16.2416423591954739   T   T   T
  2.4235563136428953  1.3282643404256897 20.6883808104416538   T   T   T
  0.0291593355749563  2.7121455174440863 11.8834768182986377   F   F   F
  1.5137229272725468 -0.0556303829029206 11.0348070799988349   F   F   F
  3.8951641890436886  1.3283445685071833 15.4080746060113967   T   T   T
  1.5094553459301714  2.7305415028938547 19.7752278643687021   T   T   T
  0.7614341235973506  1.2174144138215932 17.5847528364575112   T   T   T
  3.1596250700557684  2.6596306898585667  8.8712015584813955   F   F   F
  0.7609283799024609  3.9864570511834034 13.2250185171475483   F   F   F
 -0.7211716530913767  1.2267972473494415 11.0371856277262967   F   F   F
  1.6870251184764786  2.6010147271928963 15.4073308631673687   T   T   T
 -0.7331780046417501  3.9906735341340984 19.7753754884697805   T   T   T
  3.3500274402732195 -0.0582545581702333 17.5846354077832281   T   T   T
  0.9366237111311351  1.2725878994926449  8.8494658732768272   F   F   F
 -1.4453225013191369  2.7147930379849123 13.2250148374957792   F   F   F
  1.6947990130629129  2.8153003801747123 11.0407582029264013   F   F   F
  1.6886936071432961  0.0530875291718930 15.4082931715273723   T   T   T
 -0.7032217023775847  1.4183981034687794 19.7744896524305211   T   T   T
 -1.6386499939891470  2.8218065138737951 17.5846231272457523   T   T   T
  3.2279547937294235 -0.0003049612593239  8.9135372731794220   F   F   F
  0.7596718129077398  1.4372961580926580 13.2221143204608840   F   F   F
  0.0248113534352786  2.7136413105662669 21.0495729981035780   T   T   T
  3.3872110873490402  2.2028502887685146 22.1194253470112336   T   T   T
  1.1838559254285745  1.7236428872947889 22.1196640506306359   T   T   T
  2.7025803954362941  0.0576095714413112 22.1192216292981101   T   T   T
  0.4195130384143357  2.1131364545026670  8.8276013437729759   F   F   F
  2.6762267799228221  2.5240274532366351  8.0391937587954807   F   F   F
  3.1648900513596718  0.3116792765633036  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Pt E_tot= -76.27530903 eV
 D3-zero damping= -6.656523 eV, D3-BJ damping= -6.9253747 eV
Pt
 1.0000000000000000
     4.7985659889076251    0.0000000000000000    0.0000000000000000
     2.3992829944538125    4.1556800481299989    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.8578987326980325
  12
Cartesian
  5.5983072969349434  1.3852552135053127 10.2998504961580259
  5.5983074313317642  4.1557085677605325 10.2998504960837671
  4.7982295282700358  2.7705754626834769 14.8578987326980325
  2.3997061748454844  1.3850260679897639  8.0000000924258732
  3.1990242999908638  2.7704820195253261 10.2998506747447713
  1.5995237438406782  2.7704292760624218 12.5569129382707025
  2.3989465070371874  1.3853489325836321 14.8578986958401522
  4.7989891555223521 -0.0002006601011906  8.0000000260745274
  2.3989465337284495  4.1558020361918420 14.8578985860271295
  3.9988067642492564  1.3852026030788183 12.5569129227630683
  4.7989891692992996  2.7702525991105218  8.0000000000000000
  3.9988067717429701  4.1556559493417504 12.5569129196091431

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt3/Pd E_tot= -323.97408594 eV
 D3-zero damping= -10.8010515 eV, D3-BJ damping= -13.7979659 eV
Al  O Al  O  H Pd
 1.0000000000000000
     4.7596431118965139    0.0000000000000000    0.0000000000000000
    -2.3798215559482561    4.1219718478500011    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.6209207051251013
  11  18   1   3   3  12
Selective dynamics
Cartesian
  0.0234194810684289 -0.0592784371031871 12.3918657751636392   F   F   F
  2.4049158611375456  1.3155933415108521 16.7385837662276309   T   T   T
```

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  0.0261305310865410 -0.0590569016930196 18.9430849680374394   T   T   T
  2.4053470972324620  1.3146578705733516 10.0985295441362890   F   F   F
  0.0233302053535788  2.6911363047142571 14.5561856244294301   F   F   F
  0.0566701063245567 -0.0453725048910357  9.7781175373791616   F   F   F
  2.4041568675256215  1.3176885383056181 14.0665571956713524   F   F   F
  0.0257031667998933  2.6900771986439125 18.4156069008443772   T   T   T
  0.0245843411343020 -0.0579355167686190 16.2599417965664266   T   T   T
  2.4067734534155822  1.3140280530804211 20.7542650911081523   T   T   T
  0.0289228138234719  2.6901463396364380 11.8834768182986377   F   F   F
  1.5014445817286228 -0.0551791450629457 11.0348070799988349   F   F   F
  3.8656438745079709  1.3164140105706827 15.4065384292000811   T   T   T
  1.4988256561412714  2.6730128992900593 19.7749643875773593   T   T   T
  0.7550418070451415  1.2057330673948676 17.5901427990112751   T   T   T
  3.1339962262955097  2.6380574785125850  8.8712015584813955   F   F   F
  0.7547562189248540  3.9541214788745167 13.2250185171475483   F   F   F
 -0.7153219730782097  1.2168462581400543 11.0371856277262967   F   F   F
  1.6735205228542251  2.5820992885649576 15.4061702425443787   T   T   T
 -0.6959705772699575  3.9717261621096536 19.7743027105438962   T   T   T
  3.3261928453734662 -0.0582967066678994 17.5895537887188134   T   T   T
  0.9290264227749220  1.2622654860023896  8.8494658732768272   F   F   F
 -1.4335989759804673  2.6927723851956480 13.2250148374957792   F   F   F
  1.6810518949246007  2.7924644765526345 11.0407582029264013   F   F   F
  1.6733804054727448  0.0518171328432278 15.4066717491244294   T   T   T
 -0.7236041057790249  1.4217040939696788 19.7746402603409628   T   T   T
 -1.6247781930027916  2.8004125169632417 17.5896280017733453   T   T   T
  3.2017717032552713 -0.0003024876099842  8.9135372731794220   F   F   F
  0.7535098443923609  1.4256377372812525 13.2221143204608840   F   F   F
  0.0266880932317722  2.6883250104100882 21.0151889820920239   T   T   T
  3.2011611394808392  2.6075883359525913 21.9169909320936291   T   T   T
  0.8890065898086403  1.3550951927340003 21.9165296687659712   T   T   T
  3.1302766020096495 -0.0212171108520295 21.9166014372686320   T   T   T
  0.4161102188143752  2.0959960524499639  8.8276013437729759   F   F   F
  2.6545189517821712  2.5035541680172395  8.0391937587954807   F   F   F
  3.1392185014617393  0.3091511349942123  8.0000000000000000   F   F   F
 -0.7632779225733557  4.0495613664248813 26.0879719763469211   T   T   T
  0.0336791936577708  2.6739137093130747 28.3408229190106127   T   T   T
  3.1990596148112980  2.6721984010565292 23.8519976767918358   T   T   T
  1.6160707640444254  2.6808245679423104 26.0879300871791173   T   T   T
  2.4134730441858374  1.2999942636302650 28.3356962429478756   T   T   T
  3.2081284402838008  2.6687900062064687 30.6216356701992822   T   T   T
  0.8297215256442626  1.2919707967995917 30.6216740283927109   T   T   T
  5.5926303651925187  1.3123104634539744 23.8513367362466759   T   T   T
  1.6214336374547824  5.4261350092326435 26.0879723338353031   T   T   T
  2.4136884972518344  4.0477247753402157 28.3237993198125615   T   T   T
  0.8136355617829195  4.0652939768297989 23.8513933654157242   T   T   T
  0.8310325140534626  4.0424495475697322 30.6217052403037080   T   T   T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Pd E_tot= -272.45423668 eV
 D3-zero damping= -4.6333001 eV, D3-BJ damping= -6.7947531 eV
Al  O Al  O  H
 1.0000000000000000
     4.7596431118965130    0.0000000000000000    0.0000000000000000
    -2.3798215559482556    4.1219718478500011    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.8055094730076817
  11  18   1   3   6
Selective dynamics
Cartesian
  0.0234194810684289 -0.0592784371031871 12.3918657751636392   F   F   F
  2.4029292094959525  1.3169825759680693 16.7389943575415856   T   T   T
  0.0235355622537429 -0.0584671356138812 18.9266773274985205   T   T   T
  2.4053470972324611  1.3146578705733516 10.0985295441362890   F   F   F
  0.0233302053535788  2.6911363047142571 14.5561856244294301   F   F   F
  0.0566701063245567 -0.0453725048910357  9.7781175373791616   F   F   F
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  2.4041568675256211  1.3176885383056178 14.0665571956713524   F   F   F
  0.0232932564454556  2.6920449103150386 18.4325694729211023   T   T   T
  0.0240528568435875 -0.0567874914017225 16.2574812385891505   T   T   T
  2.4114378223828705  1.3106840918408749 20.7191842680594078   T   T   T
  0.0289228138234719  2.6901463396364385 11.8834768182986377   F   F   F
  1.5014445817286226 -0.0551791450629457 11.0348070799988349   F   F   F
  3.8647398659481205  1.3164894508166476 15.4068928927854571   T   T   T
  1.5005979478281484  2.6807180200997336 19.7798275414983742   T   T   T
  0.7521918606345439  1.2085260358851406 17.5924055860108943   T   T   T
  3.1339962262955088  2.6380574785125854  8.8712015584813955   F   F   F
  0.7547562189248538  3.9541214788745167 13.2250185171475483   F   F   F
 -0.7153219730782095  1.2168462581400545 11.0371856277262967   F   F   F
  1.6730158365266836  2.5825755805972084 15.4067585076789211   T   T   T
 -0.7151286627355163  3.9609620920410076 19.7862946289227146   T   T   T
  3.3219144680493042 -0.0572418588658301 17.5933274327492377   T   T   T
  0.9290264227749219  1.2622654860023899  8.8494658732768272   F   F   F
 -1.4335989759804670  2.6927723851956484 13.2250148374957792   F   F   F
  1.6810518949246003  2.7924644765526345 11.0407582029264013   F   F   F
  1.6730040065290046  0.0527198272458576 15.4071638581548189   T   T   T
 -0.7190464140263189  1.4205666017573466 19.7852669738601605   T   T   T
 -1.6241606246741667  2.8004222178486775 17.5890549664671596   T   T   T
  3.2017717032552708 -0.0003024876099842  8.9135372731794220   F   F   F
  0.7535098443923608  1.4256377372812525 13.2221143204608840   F   F   F
  0.0262958440605477  2.6791185363208450 21.0511151921128530   T   T   T
  3.1804395583960376  2.6829254651725640 21.9527084536504411   T   T   T
  0.9756441322056949  1.4242337128137519 21.9678419377040370   T   T   T
  3.0959532661333236  0.0001795277698530 21.9500457550430923   T   T   T
  0.4161102188143751  2.0959960524499643  8.8276013437729759   F   F   F
  2.6545189517821708  2.5035541680172395  8.0391937587954807   F   F   F
  3.1392185014617389  0.3091511349942123  8.0000000000000000   F   F   F
  3.1546065739009834  2.2147386802925109 22.8053294146809087   T   T   T
  0.7643780703042955  0.5240904602271445 22.2695162636995292   T   T   T
  4.0450460928001224 -0.2291176547821709 21.9919932480564171   T   T   T

Oxidized reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Pd E_tot= -252.83962748
eV
 D3-zero damping= -4.3513224 eV, D3-BJ damping= -6.4877449 eV
Al  O Al  O  H
 1.0000000000000000
     4.7596431118965130    0.0000000000000000    0.0000000000000000
    -2.3798215559482556    4.1219718478500011    0.0000000000000000
     0.0000000000000018    0.0000000000000032   29.8754197198952873
  11  18   1   3   3
Selective dynamics
Cartesian
  0.0234194810684289 -0.0592784371031871 12.3918657751636392   F   F   F
  2.4032911902088525  1.3160979649181272 16.7381796084239589   T   T   T
  0.0233470221764835 -0.0574459499385528 18.9266958159701311   T   T   T
  2.4053470972324611  1.3146578705733516 10.0985295441362890   F   F   F
  0.0233302053535788  2.6911363047142571 14.5561856244294301   F   F   F
  0.0566701063245567 -0.0453725048910357  9.7781175373791616   F   F   F
  2.4041568675256211  1.3176885383056178 14.0665571956713524   F   F   F
  0.0233135104648248  2.6906850487683029 18.4364410854099248   T   T   T
  0.0236854932487522 -0.0572429553392802 16.2568224051139971   T   T   T
  2.4031615316006829  1.3169689651800998 20.7165218208884596   T   T   T
  0.0289228138234719  2.6901463396364385 11.8834768182986377   F   F   F
  1.5014445817286226 -0.0551791450629457 11.0348070799988349   F   F   F
  3.8649198536234839  1.3171572026552889 15.4133073583022107   T   T   T
  1.4985866648919188  2.7066605623419417 19.7974050021591097   T   T   T
  0.7555642502065861  1.2092897362347508 17.5985728926865406   T   T   T
  3.1339962262955088  2.6380574785125854  8.8712015584813955   F   F   F
  0.7547562189248538  3.9541214788745167 13.2250185171475483   F   F   F
 -0.7153219730782095  1.2168462581400545 11.0371856277262967   F   F   F
```

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  1.6724137113935615  2.5819820845806354 15.4128326086626739   T   T   T
 -0.7278719366097617  3.9606748678345931 19.7971301868323089   T   T   T
  3.3201605327243482 -0.0570099811942726 17.5986489562989235   T   T   T
  0.9290264227749219  1.2622654860023899  8.8494658732768272   F   F   F
 -1.4335989759804670  2.6927723851956484 13.2250148374957792   F   F   F
  1.6810518949246003  2.7924644765526345 11.0407582029264013   F   F   F
  1.6731370636944289  0.0514482790603090 15.4134942873298293   T   T   T
 -0.7006583374937582  1.4052867747867568 19.7970091008328026   T   T   T
 -1.6255765239909137  2.7972421558291116 17.5984811173553126   T   T   T
  3.2017717032552708 -0.0003024876099842  8.9135372731794220   F   F   F
  0.7535098443923608  1.4256377372812525 13.2221143204608840   F   F   F
  0.0234636847335098  2.6909331082275161 21.0706123535431722   T   T   T
  3.3579586481744617  2.1909957329765870 22.1519060244088308   T   T   T
  1.1687594133373727  1.7070333036693031 22.1521224497825777   T   T   T
  2.6832983105045112  0.0539690626535243 22.1516573738212266   T   T   T
  0.4161102188143751  2.0959960524499643  8.8276013437729759   F   F   F
  2.6545189517821708  2.5035541680172395  8.0391937587954807   F   F   F
  3.1392185014617389  0.3091511349942123  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Pd E_tot= -64.29714241 eV
 D3-zero damping= -5.0028266 eV, D3-BJ damping= -5.9926421 eV
Pd
 1.0000000000000000
     4.7596431118965139    0.0000000000000000    0.0000000000000000
     2.3798215559482570    4.1219718478499994    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.7848903884610010
  12
Cartesian
  5.5528479283914560  1.3740570459520898 10.2714814415853564
  5.5528478576845748  4.1220382274812941 10.2714814507388983
  4.7598719492758716  2.7477511759738831 14.7899051002088111
  2.3796565062376036  1.3741627216645931  7.9952165569729852
  3.1730263569992152  2.7480476230114292 10.2714814199414946
  1.5866213038474464  2.7478993259487812 12.5134848823296938
  2.3800503095200480  1.3737604481566712 14.7899051261311438
  4.7594781402739592  0.0001719974450671  7.9952167919358681
  2.3800503756470106  4.1217416873580719 14.7899051069846621
  3.9664429230374592  1.3739088333168670 12.5134848944659272
  4.7594779786971992  2.7481532487407856  7.9952165411015388
  3.9664428634001498  4.1218900641908380 12.5134849084948332

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ni E_tot= -307.71698965 eV
 D3-zero damping= -9.8093496 eV, D3-BJ damping= -13.4000084 eV
Al  O Al  O  H Ni
 1.0000000000000000
     4.2502068721891444    0.0000000000000000    0.0000000000000000
    -2.1251034360945713    3.6807871226550004    0.0000000000000000
     0.0000000000000023    0.0000000000000040   38.1600250080930579
  11  18   1   3   3  12
Selective dynamics
Cartesian
  0.0209128367484845 -0.0529337210428383 12.3918657751636392   F   F   F
  2.1461225110027531  1.1779430026716082 16.7776609847381728   T   T   T
  0.0215759972200087 -0.0491012027993685 19.1016763488141663   T   T   T
  2.1478969162845702  1.1739468243159938 10.0985295441362890   F   F   F
  0.0208331164316760  2.4030974061281518 14.5561856244294301   F   F   F
  0.0506045662848760 -0.0405161747556899  9.7781175373791616   F   F   F
  2.1468340797733934  1.1766531122708206 14.0665571956713524   F   F   F
  0.0213183107043343  2.4050712722002037 18.7653451681740187   T   T   T
  0.0211173324935037 -0.0494024476926255 16.4783001325709755   T   T   T
  2.1473333209270193  1.1768450258056167 21.1437379316514793   T   T   T
  0.0258271343429752  2.4022133994330996 11.8834768182986377   F   F   F
  1.3407412970783461 -0.0492731862525310 11.0348070799988367   F   F   F
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  3.4780477236826206  1.1608304240952561 15.4770534970449649   T   T   T
  1.3706970333769604  2.3906417979359316 20.0865018787138325   T   T   T
  0.6937450636719275  1.1119737334053741 17.7830597419886196   T   T   T
  2.7985569474994767  2.3556997364738428  8.8712015584813972   F   F   F
  0.6739728154163453  3.5309021890691232 13.2250185171475483   F   F   F
 -0.6387593133203401  1.0866042279131609 11.0371856277262967   F   F   F
  1.4943677974877145  2.3389495824276447 15.4766892995174139   T   T   T
 -0.6409404314744362  3.5795842981474286 20.0864371935701804   T   T   T
  2.9298281020349242 -0.0465461592361620 17.7831664402550018   T   T   T
  0.8295904532535301  1.1271621247662933  8.8494658732768290   F   F   F
 -1.2801573723975421  2.4045583729153637 13.2250148374957792   F   F   F
  1.5011248003987880  2.4935801759848673 11.0407582029264031   F   F   F
  1.4662345760149134  0.0319676509875471 15.4768318653794523   T   T   T
 -0.6650334278268789  1.2434173846815826 20.0858159896341633   T   T   T
 -1.4351180368419130  2.4691261874968626 17.7830425756358501   T   T   T
  2.8590782494475753 -0.0002701116214981  8.9135372731794238   F   F   F
  0.6728598433974806  1.2730482445417235 13.2221143204608840   F   F   F
  0.0221147984542162  2.4033951721657161 21.3521396648475026   T   T   T
  2.8097169619785389  2.3971268944723896 22.3767769216912420   T   T   T
  0.7576623300126126  1.1355536062862266 22.3751409076893069   T   T   T
  2.8777501371594427 -0.0095015722390890 22.3755883341942763   T   T   T
  0.3715729246952494  1.8716564701958367  8.8276013437729777   F   F   F
  2.3703992980106889  2.2355926441646203  8.0391937587954825   F   F   F
  2.8032202697860775  0.2760619331338732  8.0000000000000018   F   F   F
 -0.6703894937616414  3.6053033605064790 26.1884538179753505   T   T   T
  0.0387626204924066  2.3751762845970363 28.2069615792544788   T   T   T
  2.8588845022865348  2.3840096408408691 24.1823032011534380   T   T   T
  1.4524135667120970  2.3784588275154706 26.1880233486125249   T   T   T
  2.1636860654307766  1.1483050050793959 28.2084459970859136   T   T   T
  2.8773249556325555  2.3771306632027720 30.2225062180470729   T   T   T
  0.7523853295506899  1.1528636488535704 30.2224080690679635   T   T   T
  4.9924057183123374  1.1524629670683662 24.1809497799561157   T   T   T
  1.4535295447873957  4.8340142150826688 26.1883433393187808   T   T   T
  2.1633670015362818  3.6023076787084354 28.2118693289637825   T   T   T
  0.7414769151366494  3.6164074376477835 24.1807216171804811   T   T   T
  0.7490447037483877  3.6044995493176684 30.2219200028934445   T   T   T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ni E_tot= -254.09925094 eV
 D3-zero damping= -5.5845284 eV, D3-BJ damping= -8.3455209 eV
Al  O Al  O  H
 1.0000000000000000
     4.2502068721891453    0.0000000000000000    0.0000000000000000
    -2.1251034360945718    3.6807871226550009    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.7384898915196381
  11  18   1   3   6
Selective dynamics
Cartesian
  0.0209128367484845 -0.0529337210428383 12.3918657751636392   F   F   F
  2.1464686855775938  1.1777540833374802 16.7780194968538758   T   T   T
  0.0202006449999016 -0.0500694347129976 19.0961335731590012   T   T   T
  2.1478969162845707  1.1739468243159938 10.0985295441362890   F   F   F
  0.0208331164316760  2.4030974061281514 14.5561856244294301   F   F   F
  0.0506045662848760 -0.0405161747556899  9.7781175373791616   F   F   F
  2.1468340797733938  1.1766531122708208 14.0665571956713524   F   F   F
  0.0206187546974648  2.4046612702031847 18.7716619457057696   T   T   T
  0.0219452883647102 -0.0496881091347346 16.4783324604576968   T   T   T
  2.1530957279522749  1.1696129900187193 21.1193890461737759   T   T   T
  0.0258271343429752  2.4022133994331001 11.8834768182986377   F   F   F
  1.3407412970783466 -0.0492731862525310 11.0348070799988349   F   F   F
  3.4789394740189312  1.1608499030588635 15.4782059641568566   T   T   T
  1.3718573607779552  2.3952201649829150 20.0915315073679750   T   T   T
  0.6945935868016595  1.1122416192467570 17.7848354129820514   T   T   T
  2.7985569474994776  2.3556997364738423  8.8712015584813955   F   F   F
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  0.6739728154163456  3.5309021890691232 13.2250185171475483   F   F   F
 -0.6387593133203404  1.0866042279131611 11.0371856277262967   F   F   F
  1.4947377550271177  2.3389025390720946 15.4770079233542788   T   T   T
 -0.6567362920281972  3.5662024154834562 20.1002874172562045   T   T   T
  2.9283136012101623 -0.0477284120541472 17.7852512169380148   T   T   T
  0.8295904532535303  1.1271621247662937  8.8494658732768272   F   F   F
 -1.2801573723975426  2.4045583729153637 13.2250148374957792   F   F   F
  1.5011248003987885  2.4935801759848673 11.0407582029264013   F   F   F
  1.4674835362177556  0.0319353470265594 15.4777613963655778   T   T   T
 -0.6627299710095291  1.2461059344602106 20.0787928815645138   T   T   T
 -1.4331820362206540  2.4690500792693255 17.7808406567407253   T   T   T
  2.8590782494475762 -0.0002701116214981  8.9135372731794220   F   F   F
  0.6728598433974808  1.2730482445417237 13.2221143204608840   F   F   F
  0.0240111865228629  2.3912309517668717 21.3740187383927243   T   T   T
  2.8279535141912695  2.4502751504676294 22.4382508339092794   T   T   T
  0.8215341979689265  1.2384592646450532 22.4069709706094358   T   T   T
  2.8321050466461091  0.0250302644696759 22.3708250608471317   T   T   T
  0.3715729246952496  1.8716564701958369  8.8276013437729759   F   F   F
  2.3703992980106898  2.2355926441646203  8.0391937587954807   F   F   F
  2.8032202697860789  0.2760619331338732  8.0000000000000000   F   F   F
  2.8733162018167109  1.7902761286955444 23.1545369204272689   T   T   T
  0.7959717820439172  0.3246737799438781 22.7430671925474428   T   T   T
  3.7288437792933853 -0.3700889082053031 22.4824525941304962   T   T   T

Oxidized reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ni E_tot= -236.80559363
eV
 D3-zero damping= -5.2981976 eV, D3-BJ damping= -8.0119913 eV
Al  O Al  O  H
 1.0000000000000000
     4.2502068721891453    0.0000000000000000    0.0000000000000000
    -2.1251034360945718    3.6807871226550009    0.0000000000000000
     0.0000000000000018    0.0000000000000032   29.8754197198952873
  11  18   1   3   3
Selective dynamics
Cartesian
  0.0209128367484845 -0.0529337210428383 12.3918657751636392   F   F   F
  2.1468598369279568  1.1756997982986923 16.7787418545576728   T   T   T
  0.0187401114874141 -0.0547357168442107 19.1034539046521026   T   T   T
  2.1478969162845707  1.1739468243159938 10.0985295441362890   F   F   F
  0.0208331164316760  2.4030974061281514 14.5561856244294301   F   F   F
  0.0506045662848760 -0.0405161747556899  9.7781175373791616   F   F   F
  2.1468340797733938  1.1766531122708208 14.0665571956713524   F   F   F
  0.0202036071811104  2.3995012981861512 18.7761967975019708   T   T   T
  0.0213587857488330 -0.0506142246576394 16.4813288865747793   T   T   T
  2.1408590848030813  1.1951913169379442 21.0696705470537680   T   T   T
  0.0258271343429752  2.4022133994331001 11.8834768182986377   F   F   F
  1.3407412970783466 -0.0492731862525310 11.0348070799988349   F   F   F
  3.4791989414472955  1.1616504484246906 15.4834890783510879   T   T   T
  1.3330921375069260  2.4186332420392516 20.1132959560877502   T   T   T
  0.7006831682857358  1.1060643312903624 17.7951427824016548   T   T   T
  2.7985569474994776  2.3556997364738423  8.8712015584813955   F   F   F
  0.6739728154163456  3.5309021890691232 13.2250185171475483   F   F   F
 -0.6387593133203404  1.0866042279131611 11.0371856277262967   F   F   F
  1.4935805077470352  2.3377168090480662 15.4816388078888387   T   T   T
 -0.6567391093870524  3.5604368215956175 20.1392242988496939   T   T   T
  2.9260280806855059 -0.0528742741625124 17.7866248161542622   T   T   T
  0.8295904532535303  1.1271621247662937  8.8494658732768272   F   F   F
 -1.2801573723975426  2.4045583729153637 13.2250148374957792   F   F   F
  1.5011248003987885  2.4935801759848673 11.0407582029264013   F   F   F
  1.4663144443036011  0.0305473897715759 15.4807073485597755   T   T   T
 -0.6716336756852185  1.2507106191475001 20.0432429529036540   T   T   T
 -1.4376417219178548  2.4669750592955859 17.7937382057382187   T   T   T
  2.8590782494475762 -0.0002701116214981  8.9135372731794220   F   F   F
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  0.6728598433974808  1.2730482445417237 13.2221143204608840   F   F   F
 -0.0198083954428825  2.3815798353842621 21.4549074470083454   T   T   T
  2.7350808075564514  2.1857114831906128 22.4155264395779739   T   T   T
  0.6921720676309528  0.9973614707741593 22.4024479248371975   T   T   T
  3.6470502619667911  0.2226094885725856 22.4872793491318568   T   T   T
  0.3715729246952496  1.8716564701958369  8.8276013437729759   F   F   F
  2.3703992980106898  2.2355926441646203  8.0391937587954807   F   F   F
  2.8032202697860789  0.2760619331338732  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ni E_tot= -65.21703902 eV
 D3-zero damping= -3.420018 eV, D3-BJ damping= -4.2254943 eV
Ni
 1.0000000000000000
     4.2502068721891444    0.0000000000000000    0.0000000000000000
     2.1251034360945722    3.6807871226549991    0.0000000000000000
     0.0000000000000000    0.0000000000000000   21.9758133853619810
  12
Cartesian
  4.9585061929312291  1.2270017851453026  9.9895998775674695
  4.9585061771093297  3.6808598584578669  9.9895998323622592
  4.2502059509158636  2.4538638921055140 13.9944372090852251
  2.1251717187803290  1.2268560216223283  7.9811999905978519
  2.8334027408703193  2.4539307580759346  9.9895998825781707
  1.4167980955638388  2.4537872830549721 11.9861271711918747
  2.1251024736007613  1.2269348309401560 13.9944371989874536
  4.2502751608257947 -0.0000730266200595  7.9812000981523132
  2.1251025104935892  3.6807929337745535 13.9944373017538730
  3.5419015386852264  1.2268581946858119 11.9861272515067103
  4.2502751548749025  2.4537850453326344  7.9811999479367666
  3.5419015147887558  3.6807163213213938 11.9861272036044095

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ir E_tot= -368.4846307 eV
 D3-zero damping= -11.9571789 eV, D3-BJ damping= -14.5429929 eV
Al  O Al  O  H Ir
 1.0000000000000000
     4.7026274333618803    0.0000000000000000    0.0000000000000000
    -2.3513137166809392    4.0725948218250014    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.5053890400289589
  11  18   1   3   3  12
Selective dynamics
Cartesian
  0.0231389395293568 -0.0585683417799761 12.3918657751636410   F   F   F
  2.3755263492794794  1.2985950517408729 16.7410652877857622   T   T   T
  0.0253854016116128 -0.0611870733673251 18.9589520177835134   T   T   T
  2.3765334879689353  1.2989096077793856 10.0985295441362908   F   F   F
  0.0230507332466761  2.6588992317162918 14.5561856244294319   F   F   F
  0.0559912561484482 -0.0448289884776491  9.7781175373791633   F   F   F
  2.3753575160021723  1.3019039711978397 14.0665571956713542   F   F   F
  0.0246647928292756  2.6548465077578851 18.4466208118656887   T   T   T
  0.0239762289298689 -0.0580402791621980 16.2811663941789320   T   T   T
  2.3781038695827301  1.2956741725232217 20.7825234983181488   T   T   T
  0.0285763479611146  2.6579211254121899 11.8834768182986394   F   F   F
  1.4834588043085810 -0.0545181550847557 11.0348070799988367   F   F   F
  3.8220023254681554  1.2986826641919014 15.4150719457840939   T   T   T
  1.4847822499774932  2.6357782241864562 19.8069476086614067   T   T   T
  0.7472913808509360  1.1912986726857491 17.6095504026949357   T   T   T
  3.0964541423269449  2.6064562358112546  8.8712015584813972   F   F   F
  0.7457150078637397  3.9067551293759784 13.2250185171475501   F   F   F
 -0.7067531441330630  1.2022696788778879 11.0371856277262985   F   F   F
  1.6530246379769364  2.5532812737071731 15.4147110354012362   T   T   T
 -0.6882013511509386  3.9253284558297268 19.8071576468964068   T   T   T
  3.2824984841186864 -0.0593954363622726 17.6093046868955199   T   T   T
  0.9178976321017891  1.2471448306332105  8.8494658732768290   F   F   F
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 -1.4164259198414928  2.6605157136192621 13.2250148374957810   F   F   F
  1.6609146047564587  2.7590135952215196 11.0407582029264031   F   F   F
  1.6507121283022943  0.0485424814466422 15.4153683410441804   T   T   T
 -0.7184687705110759  1.3992009178894294 19.8071322192585555   T   T   T
 -1.6045153656305871  2.7618361942829477 17.6093242666870005   T   T   T
  3.1634177380771238 -0.0002988641163890  8.9135372731794238   F   F   F
  0.7444835636291719  1.4085600486763012 13.2221143204608858   F   F   F
  0.0270030181758108  2.6530639739022233 21.0387297734247767   T   T   T
  3.1657822136749565  2.5729141089382082 21.9810416562121773   T   T   T
  0.8795644048868761  1.3392859157718213 21.9809769719859354   T   T   T
  3.0913866582277545 -0.0242755132996939 21.9806118606185379   T   T   T
  0.4111256420481892  2.0708881537426742  8.8276013437729777   F   F   F
  2.6227205173910266  2.4735641380334923  8.0391937587954825   F   F   F
  3.1016138599536500  0.3054478191537051  8.0000000000000018   F   F   F
 -0.7562943665347014  4.0107779545408482 26.0834249590008476   T   T   T
  0.0304338390249515  2.6552043030295889 28.3246588780665327   T   T   T
  3.1645154506347981  2.6402038727999524 23.9184385099815167   T   T   T
  1.5970963419405149  2.6578559880019550 26.0834536932171446   T   T   T
  2.3818075712380402  1.2976912383129318 28.3289883440211483   T   T   T
  3.1667601159270693  2.6556376688669547 30.5052916686003890   T   T   T
  0.8134866954197093  1.2984911827804071 30.5052626981275274   T   T   T
  5.5276471798489837  1.3042297926852373 23.9185602265176307   T   T   T
  1.5998668794655393  5.3687119172494899 26.0834625552451165   T   T   T
  2.3818140523193194  4.0127407233587968 28.3216168181875965   T   T   T
  0.8005491424281785  4.0189865253670476 23.9182332701201261   T   T   T
  0.8141647943528620  4.0116769307668942 30.5052368848678839   T   T   T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ir E_tot= -271.99084195 eV
 D3-zero damping= -4.7375645 eV, D3-BJ damping= -6.9438126 eV
Al  O Al  O  H
 1.0000000000000000
     4.7026274333618803    0.0000000000000000    0.0000000000000000
    -2.3513137166809392    4.0725948218250014    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.8473266041151071
  11  18   1   3   6
Selective dynamics
Cartesian
  0.0231389395293568 -0.0585683417799761 12.3918657751636392   F   F   F
  2.3743160698300874  1.3026152564160409 16.7439134635603608   T   T   T
  0.0230006825895793 -0.0552247117803561 18.9484841239901840   T   T   T
  2.3765334879689357  1.2989096077793856 10.0985295441362890   F   F   F
  0.0230507332466761  2.6588992317162923 14.5561856244294301   F   F   F
  0.0559912561484482 -0.0448289884776491  9.7781175373791616   F   F   F
  2.3753575160021723  1.3019039711978397 14.0665571956713524   F   F   F
  0.0228171960088817  2.6614060242679338 18.4709093408417466   T   T   T
  0.0237565255171129 -0.0554780694824012 16.2824922375780687   T   T   T
  2.3819064544411797  1.2968470957939517 20.7635598943729534   T   T   T
  0.0285763479611146  2.6579211254121904 11.8834768182986377   F   F   F
  1.4834588043085810 -0.0545181550847557 11.0348070799988349   F   F   F
  3.8217610865567693  1.2998602367636722 15.4153541406318713   T   T   T
  1.4855784174806976  2.6500534768254993 19.8157142401200268   T   T   T
  0.7453656438758971  1.1986334109748458 17.6147498505700817   T   T   T
  3.0964541423269449  2.6064562358112546  8.8712015584813955   F   F   F
  0.7457150078637397  3.9067551293759788 13.2250185171475483   F   F   F
 -0.7067531441330630  1.2022696788778879 11.0371856277262967   F   F   F
  1.6528156852389657  2.5551886832590354 15.4152524916619953   T   T   T
 -0.7075118739920906  3.9189144830327289 19.8224125412552183   T   T   T
  3.2786746852112523 -0.0547078357926943 17.6155666006377523   T   T   T
  0.9178976321017891  1.2471448306332105  8.8494658732768272   F   F   F
 -1.4164259198414928  2.6605157136192625 13.2250148374957792   F   F   F
  1.6609146047564589  2.7590135952215200 11.0407582029264013   F   F   F
  1.6507692924343522  0.0502261391861390 15.4159901146254050   T   T   T
 -0.7127979569945549  1.4042269103987348 19.8198969534343732   T   T   T
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 -1.6033059612063061  2.7654477415761276 17.6112252410927965   T   T   T
  3.1634177380771238 -0.0002988641163890  8.9135372731794220   F   F   F
  0.7444835636291720  1.4085600486763012 13.2221143204608840   F   F   F
  0.0262294226795711  2.6485625642882558 21.0901270413769382   T   T   T
  3.1354423976054711  2.6675621711701316 22.0036140591830467   T   T   T
  0.9579256965674069  1.4020348058521013 22.0189388598919713   T   T   T
  3.0697246894512271  0.0059672804903616 21.9978412399462719   T   T   T
  0.4111256420481892  2.0708881537426742  8.8276013437729759   F   F   F
  2.6227205173910266  2.4735641380334923  8.0391937587954807   F   F   F
  3.1016138599536500  0.3054478191537051  8.0000000000000000   F   F   F
  3.1144920243376282  2.1827417108265030 22.8473585041151033   T   T   T
  0.7648072188890207  0.4956609058806796 22.3155280779227034   T   T   T
  4.0153283081441487 -0.2401056959673748 22.0381429845354049   T   T   T

Oxidized reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ir E_tot= -252.51211109
eV
 D3-zero damping= -4.4547936 eV, D3-BJ damping= -6.6336026 eV
Al  O Al  O  H
 1.0000000000000000
     4.7026274333618803    0.0000000000000000    0.0000000000000000
    -2.3513137166809392    4.0725948218250014    0.0000000000000000
     0.0000000000000018    0.0000000000000032   29.8754197198952873
  11  18   1   3   3
Selective dynamics
Cartesian
  0.0231389395293568 -0.0585683417799761 12.3918657751636392   F   F   F
  2.3749271881601794  1.3004064469820913 16.7417987800941184   T   T   T
  0.0239484831834601 -0.0561022545741185 18.9437568122948363   T   T   T
  2.3765334879689357  1.2989096077793856 10.0985295441362890   F   F   F
  0.0230507332466761  2.6588992317162923 14.5561856244294301   F   F   F
  0.0559912561484482 -0.0448289884776491  9.7781175373791616   F   F   F
  2.3753575160021723  1.3019039711978397 14.0665571956713524   F   F   F
  0.0234814224297204  2.6587653551547663 18.4696405066897889   T   T   T
  0.0234823678293924 -0.0565785889429491 16.2788206685472439   T   T   T
  2.3753066063131225  1.3024707471367469 20.7575836706554249   T   T   T
  0.0285763479611146  2.6579211254121904 11.8834768182986377   F   F   F
  1.4834588043085810 -0.0545181550847557 11.0348070799988349   F   F   F
  3.8216266617585548  1.3004249224831550 15.4203549002711018   T   T   T
  1.4849012706768774  2.6731209380066261 19.8277809356684962   T   T   T
  0.7485846785919943  1.1977385382046859 17.6174459755262696   T   T   T
  3.0964541423269449  2.6064562358112546  8.8712015584813955   F   F   F
  0.7457150078637397  3.9067551293759788 13.2250185171475483   F   F   F
 -0.7067531441330630  1.2022696788778879 11.0371856277262967   F   F   F
  1.6520914776394782  2.5538474920955547 15.4201936857224222   T   T   T
 -0.7182352646711658  3.9180137785814240 19.8277747005756240   T   T   T
  3.2777277699843346 -0.0557378104716819 17.6177190334000748   T   T   T
  0.9178976321017891  1.2471448306332105  8.8494658732768272   F   F   F
 -1.4164259198414928  2.6605157136192625 13.2250148374957792   F   F   F
  1.6609146047564589  2.7590135952215200 11.0407582029264013   F   F   F
  1.6511701746326999  0.0488126071475922 15.4208471394359332   T   T   T
 -0.6946417033274688  1.3874253367109177 19.8276717836330363   T   T   T
 -1.6040675536046847  2.7610897642989505 17.6173599065309965   T   T   T
  3.1634177380771238 -0.0002988641163890  8.9135372731794220   F   F   F
  0.7444835636291720  1.4085600486763012 13.2221143204608840   F   F   F
  0.0243221322637566  2.6599993337834404 21.1002529874371056   T   T   T
  3.3182056813710639  2.1757781218980687 22.1977846687154141   T   T   T
  1.1489708281467186  1.6838370227302875 22.1982403387869418   T   T   T
  2.6603591465989673  0.0506788524181105 22.1975287282221636   T   T   T
  0.4111256420481892  2.0708881537426742  8.8276013437729759   F   F   F
  2.6227205173910266  2.4735641380334923  8.0391937587954807   F   F   F
  3.1016138599536500  0.3054478191537051  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ir E_tot= -106.94013146 eV
```

```
 D3-zero damping= -6.1232614 eV, D3-BJ damping= -6.5235959 eV
Ir
 1.0000000000000000
     4.7026274333618803    0.0000000000000000    0.0000000000000000
     2.3513137166809401    4.0725948218249997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.5811649222271171
  12
Cartesian
  5.4864084891462452  1.3575215306337221 10.1973726642282934
  5.4864084540848266  4.0725847462958393 10.1973726356270795
  4.7026635878283853  2.7150232475461178 14.5811649222271171
  2.3513120976592536  1.3575339961453150  8.0000000423709920
  3.1350947454278209  2.7150531231366286 10.1973726499082780
  1.5675654285001861  2.7150382812561955 12.3838000721759229
  2.3513498709292273  1.3574916069474934 14.5811649118501006
  4.7026258509002323  0.0000024137672120  8.0000000000000000
  2.3513498860676845  4.0725548650549008 14.5811648828473093
  3.9188791450128124  1.3575066558559188 12.3838000305401774
  4.7026258788566748  2.7150656023433632  8.0000000435518448
  3.9188791822807461  4.0725698781837902 12.3838000612110672

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt3/Rh E_tot= -347.5159532 eV
 D3-zero damping= -10.9350715 eV, D3-BJ damping= -13.967767 eV
Al  O Al  O  H Rh
 1.0000000000000000
     4.6378478337567808    0.0000000000000000    0.0000000000000000
    -2.3189239168783895    4.0164940429200016    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.4531453496542710
  11  18   1   3   3  12
Selective dynamics
Cartesian
  0.0228201961759361 -0.0577615515794331 12.3918657751636374   F   F   F
  2.3434805816833011  1.2823448613784003 16.7469595640743769   T   T   T
  0.0246033040707563 -0.0575101014177803 18.9802031819491184   T   T   T
  2.3437962809542858  1.2810168774903075 10.0985295441362872   F   F   F
  0.0227332049518062  2.6222723821387675 14.5561856244294283   F   F   F
  0.0552199657993656 -0.0442114605179213  9.7781175373791598   F   F   F
  2.3426365082281029  1.2839699929753310 14.0665571956713507   F   F   F
  0.0246628223309164  2.6208105491436458 18.4933996735380006   T   T   T
  0.0244908986538195 -0.0562426813331224 16.3089603862560466   T   T   T
  2.3429601379284994  1.2805399445973418 20.8327157657293967   T   T   T
  0.0281827032581632  2.6213077494375923 11.8834768182986359   F   F   F
  1.4630238732545022 -0.0537671569868531 11.0348070799988349   F   F   F
  3.7730156398395178  1.2801723551642836 15.4238403562657993   T   T   T
  1.4663635411357725  2.6031399040950487 19.8463997119741684   T   T   T
  0.7398938384984968  1.1806158953233554 17.6342370704626390   T   T   T
  3.0537998894910805  2.5705517986138218  8.8712015584813955   F   F   F
  0.7354426398495907  3.8529388242099070 13.2250185171475465   F   F   F
 -0.6970174833040156  1.1857081822425095 11.0371856277262950   F   F   F
  1.6302869771352217  2.5226970287248154 15.4232733214578062   T   T   T
 -0.6817085549326969  3.8768860073190323 19.8460743172104728   T   T   T
  3.2334257256067991 -0.0560602206868448 17.6342156515270254   T   T   T
  0.9052534152403410  1.2299651701300538  8.8494658732768272   F   F   F
 -1.3969143796955150  2.6238665966918515 13.2250148374957774   F   F   F
  1.6380351858360731  2.7210076509837253 11.0407582029264013   F   F   F
  1.6256794598379838  0.0466129812803188 15.4240429142257867   T   T   T
 -0.7115369378286706  1.3797377109993820 19.8461567252493936   T   T   T
 -1.5802506255735835  2.7218311779079878 17.6339073932691690   T   T   T
  3.1198410487985933 -0.0002947472055619  8.9135372731794220   F   F   F
  0.7342281589967881  1.3891568624222377 13.2221143204608822   F   F   F
  0.0237083834458538  2.6196029860017291 21.0884433214247302   T   T   T
  3.1071010668910151  2.5514588300754193 22.0358753590145291   T   T   T
  0.8583120251325943  1.3072142458617189 22.0349953841435529   T   T   T
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```
  3.0595934050173805 -0.0175053380768489 22.0365260656913762   T   T   T
  0.4054623070601076  2.0423612701382701  8.8276013437729759   F   F   F
  2.5865920365789266  2.4394903151057870  8.0391937587954807   F   F   F
  3.0588885310126357  0.3012402165516674  7.9999999999999991   F   F   F
 -0.7565529895838085  3.9559118569691254 26.0929481162598940   T   T   T
  0.0122852087368287  2.6140550379108647 28.2933732337493602   T   T   T
  3.1060975243792495  2.6060967736657004 23.9482312528507606   T   T   T
  1.5591533404379212  2.6171126466599262 26.0927947565940563   T   T   T
  2.3317677578020697  1.2755300318729925 28.2979015171970048   T   T   T
  3.1086640678940709  2.6024758636265988 30.4522257620942511   T   T   T
  0.7896195114759923  1.2756377797982377 30.4514802680500765   T   T   T
  5.4402128980004631  1.2862382684716829 23.9466235422170293   T   T   T
  1.5615009245314109  5.2970704747424300 26.0929472322487648   T   T   T
  2.3318067541732410  3.9525141821965111 28.2942323962606110   T   T   T
  0.7801025543861463  3.9668727854049073 23.9483037831193002   T   T   T
  0.7809963728532402  3.9463614162111877 30.4520378717683933   T   T   T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Rh E_tot= -271.05619255 eV
 D3-zero damping= -4.8570982 eV, D3-BJ damping= -7.1212737 eV
Al  O Al  O  H
 1.0000000000000000
     4.6378478337567808    0.0000000000000000    0.0000000000000000
    -2.3189239168783895    4.0164940429200007    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.8909939930185153
  11  18   1   3   6
Selective dynamics
Cartesian
  0.0228201961759361 -0.0577615515794330 12.3918657751636392   F   F   F
  2.3410041246095163  1.2845589012782730 16.7494192950454064   T   T   T
  0.0214910090707822 -0.0540721377776474 18.9705178368257243   T   T   T
  2.3437962809542858  1.2810168774903070 10.0985295441362890   F   F   F
  0.0227332049518062  2.6222723821387666 14.5561856244294301   F   F   F
  0.0552199657993656 -0.0442114605179213  9.7781175373791616   F   F   F
  2.3426365082281029  1.2839699929753308 14.0665571956713524   F   F   F
  0.0218062309754939  2.6251722196068745 18.5128687829240981   T   T   T
  0.0229282517381014 -0.0548023125005550 16.3092405008693540   T   T   T
  2.3482863236740479  1.2796572611087591 20.8113195760041592   T   T   T
  0.0281827032581632  2.6213077494375918 11.8834768182986377   F   F   F
  1.4630238732545022 -0.0537671569868531 11.0348070799988349   F   F   F
  3.7715889243440590  1.2808060703806934 15.4241266156483032   T   T   T
  1.4672146182936137  2.6136115635933796 19.8539318927598458   T   T   T
  0.7365709355113910  1.1857456255991192 17.6388837971426682   T   T   T
  3.0537998894910801  2.5705517986138209  8.8712015584813955   F   F   F
  0.7354426398495906  3.8529388242099061 13.2250185171475483   F   F   F
 -0.6970174833040156  1.1857081822425093 11.0371856277262967   F   F   F
  1.6290820455502593  2.5237109922531458 15.4240888758219850   T   T   T
 -0.7000675576924695  3.8689617654009010 19.8608233066860151   T   T   T
  3.2286231872910873 -0.0530896422085388 17.6401145828444506   T   T   T
  0.9052534152403410  1.2299651701300536  8.8494658732768272   F   F   F
 -1.3969143796955150  2.6238665966918506 13.2250148374957792   F   F   F
  1.6380351858360729  2.7210076509837244 11.0407582029264013   F   F   F
  1.6247665879009385  0.0476922944337645 15.4245659524425438   T   T   T
 -0.7058909860088721  1.3833972140180297 19.8566459240638054   T   T   T
 -1.5805899620443948  2.7238905110241660 17.6358853023067930   T   T   T
  3.1198410487985933 -0.0002947472055619  8.9135372731794220   F   F   F
  0.7342281589967881  1.3891568624222375 13.2221143204608840   F   F   F
  0.0254789776346875  2.6127909687952613 21.1315854868124724   T   T   T
  3.0855791362448013  2.6450965408121805 22.0587770125144367   T   T   T
  0.9377339176985722  1.3778864130921042 22.0749750684514332   T   T   T
  3.0370605254176541  0.0116030329084187 22.0498191408547335   T   T   T
  0.4054623070601076  2.0423612701382692  8.8276013437729759   F   F   F
  2.5865920365789266  2.4394903151057865  8.0391937587954807   F   F   F
  3.0588885310126357  0.3012402165516673  8.0000000000000000   F   F   F
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  3.0690171393489494  2.1406424225329692 22.8910556296239278   T   T   T
  0.7653654616227846  0.4667705502868754 22.3707753549695845   T   T   T
  3.9785203241649940 -0.2520154780188070 22.0914333032315966   T   T   T

Oxidized reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Rh E_tot= -251.74830738
eV
 D3-zero damping= -4.5729794 eV, D3-BJ damping= -6.8054609 eV
Al  O Al  O  H
 1.0000000000000000
     4.6378478337567808    0.0000000000000000    0.0000000000000000
    -2.3189239168783895    4.0164940429200007    0.0000000000000000
     0.0000000000000018    0.0000000000000032   29.8754197198952873
  11  18   1   3   3
Selective dynamics
Cartesian
  0.0228201961759361 -0.0577615515794330 12.3918657751636392   F   F   F
  2.3426944906641540  1.2832151568775523 16.7463767550332783   T   T   T
  0.0240602097585842 -0.0550338958621075 18.9648029362130757   T   T   T
  2.3437962809542858  1.2810168774903070 10.0985295441362890   F   F   F
  0.0227332049518062  2.6222723821387666 14.5561856244294301   F   F   F
  0.0552199657993656 -0.0442114605179213  9.7781175373791616   F   F   F
  2.3426365082281029  1.2839699929753308 14.0665571956713524   F   F   F
  0.0241508283514455  2.6224106571433694 18.5108525375284287   T   T   T
  0.0237488802132690 -0.0556567579879170 16.3056539612425020   T   T   T
  2.3430925302832661  1.2843425983088852 20.8065360961355026   T   T   T
  0.0281827032581632  2.6213077494375918 11.8834768182986377   F   F   F
  1.4630238732545022 -0.0537671569868531 11.0348070799988349   F   F   F
  3.7722868942532668  1.2815113741570676 15.4291393359074522   T   T   T
  1.4682260904788993  2.6344026012821651 19.8645576988090937   T   T   T
  0.7405010859440405  1.1850021831979902 17.6403014252281132   T   T   T
  3.0537998894910801  2.5705517986138209  8.8712015584813955   F   F   F
  0.7354426398495906  3.8529388242099061 13.2250185171475483   F   F   F
 -0.6970174833040156  1.1857081822425093 11.0371856277262967   F   F   F
  1.6289321179383405  2.5223946142545399 15.4289450735892295   T   T   T
 -0.7083204292416295  3.8684044912876834 19.8646349338316135   T   T   T
  3.2291707033411039 -0.0542029839398598 17.6408634797747332   T   T   T
  0.9052534152403410  1.2299651701300536  8.8494658732768272   F   F   F
 -1.3969143796955150  2.6238665966918506 13.2250148374957792   F   F   F
  1.6380351858360729  2.7210076509837244 11.0407582029264013   F   F   F
  1.6260127391307015  0.0463492746378512 15.4294218460050079   T   T   T
 -0.6878607968018955  1.3659725886618648 19.8661379831379250   T   T   T
 -1.5794235533155245  2.7199614643373322 17.6405280113127745   T   T   T
  3.1198410487985933 -0.0002947472055619  8.9135372731794220   F   F   F
  0.7342281589967881  1.3891568624222375 13.2221143204608840   F   F   F
  0.0234570532155919  2.6238151954500561 21.1369533288818943   T   T   T
  3.2633478046736761  2.1689329655022771 22.2490378600044423   T   T   T
  1.1218570310974731  1.6495743283071718 22.2506690949305757   T   T   T
  2.6419421576306865  0.0455102194127464 22.2491276542647611   T   T   T
  0.4054623070601076  2.0423612701382692  8.8276013437729759   F   F   F
  2.5865920365789266  2.4394903151057865  8.0391937587954807   F   F   F
  3.0588885310126357  0.3012402165516673  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Rh E_tot= -87.43546597 eV
 D3-zero damping= -4.9774707 eV, D3-BJ damping= -5.851527 eV
Rh
 1.0000000000000000
     4.6378478337567808    0.0000000000000000    0.0000000000000000
     2.3189239168783904    4.0164940429199998    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.5017793304367331
  12
Cartesian
  5.4108142057622519  1.3387991243054735 10.1752851028337794
  5.4108141403760817  4.0164618613968379 10.1752850133523438
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  4.6379466470880759  2.6776412699707026 14.5014161875795899
  2.3188828011512301  1.3388716553935265  8.0003510262368671
  3.0918902315888106  2.6776304420597286 10.1752850060218236
  1.5459663323519763  2.6776043926790640 12.3263602656353140
  2.3190227133217634  1.3388098764875969 14.5014160636995015
  4.6378067377148673  0.0000402027084479  8.0003509285714287
  2.3190226536666607  4.0164725948344362 14.5014160673406369
  3.8648901913752267  1.3387731495742594 12.3263602581955620
  4.6378067323153296  2.6777029147935729  8.0003509576555665
  3.8648901694200579  4.0164357576330119 12.3263602750460386

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt3/Os E_tot= -394.29511923 eV
 D3-zero damping= -10.624958 eV, D3-BJ damping= -13.7034344 eV
Al  O Al  O  H Os
 1.0000000000000000
     4.6911111462397965    0.0000000000000000    0.0000000000000000
    -2.3455555731198974    4.0626214246200014    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.4709379869281420
  11  18   1   3   3  12
Selective dynamics
Cartesian
  0.0230822744681551 -0.0584249134838246 12.3918657751636410   F   F   F
  2.3706054680720530  1.2965278532899276 16.7425891896961048   T   T   T
  0.0269114527858310 -0.0591233619925935 18.9627660712234523   T   T   T
  2.3707135835877096  1.2957287017431771 10.0985295441362908   F   F   F
  0.0229942841942676  2.6523878404961625 14.5561856244294319   F   F   F
  0.0558541388897946 -0.0447192065504144  9.7781175373791633   F   F   F
  2.3695404914643969  1.2987157322505380 14.0665571956713542   F   F   F
  0.0260609833219132  2.6497861685039812 18.4559214323910332   T   T   T
  0.0244057022043301 -0.0571786991427723 16.2866902863839194   T   T   T
  2.3736930685911246  1.2940061887719683 20.7897041794221238   T   T   T
  0.0285063672040412  2.6514121294813311 11.8834768182986394   F   F   F
  1.4798259548502117 -0.0543846453104392 11.0348070799988349   F   F   F
  3.8135657396176219  1.2959064165247509 15.4170415737070989   T   T   T
  1.4838601503125235  2.6324705588258652 19.8153240091538443   T   T   T
  0.7471282133816336  1.1903103213964883 17.6145935035162360   T   T   T
  3.0888712207647515  2.6000732724980651  8.8712015584813955   F   F   F
  0.7438888227654091  3.8971878577978853 13.2250185171475501   F   F   F
 -0.7050223729317278  1.1993254348321216 11.0371856277262985   F   F   F
  1.6489933146323441  2.5480571760901154 15.4166111896045166   T   T   T
 -0.6865926713162238  3.9177689790393084 19.8153917594666389   T   T   T
  3.2747184725356497 -0.0577233833031230 17.6143618639634987   T   T   T
  0.9156497881401406  1.2440906916107350  8.8494658732768272   F   F   F
 -1.4129572275389017  2.6540003637887630 13.2250148374957810   F   F   F
  1.6568471829279845  2.7522570334512015 11.0407582029264013   F   F   F
  1.6466919980603087  0.0483063248858367 15.4172780722542733   T   T   T
 -0.7146398627540266  1.3959605542746256 19.8153608520710236   T   T   T
 -1.5991552601248626  2.7553947720613627 17.6143692043931672   T   T   T
  3.1556708290406270 -0.0002981322266053  8.9135372731794220   F   F   F
  0.7426603942205982  1.4051106191437441 13.2221143204608858   F   F   F
  0.0286619252282647  2.6478467849473319 21.0465298223525998   T   T   T
  3.1652352431769466  2.5542404269827435 22.0042937151304692   T   T   T
  0.8871370169815957  1.3476669275025788 22.0041568376589787   T   T   T
  3.0713216495364484 -0.0217546001540984 22.0039904253808629   T   T   T
  0.4101188344700492  2.0658167457023455  8.8276013437729759   F   F   F
  2.6162977243998191  2.4675066148228737  8.0391937587954807   F   F   F
  3.0940183027339434  0.3046998065084266  8.0000000000000000   F   F   F
 -0.7328175286472859  4.0021879326429648 26.0668085363276667   T   T   T
  0.0323440121546524  2.6440250640414749 28.3442212547020063   T   T   T
  3.1547694661198893  2.6366553787422538 23.9323568132513493   T   T   T
  1.5872142546717682  2.6290536840703407 26.0665463807879938   T   T   T
  2.3779581818785656  1.2899061542910628 28.3438366658304091   T   T   T
  3.1583765400698907  2.6456477772565763 30.4707230316775082   T   T   T
```

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  0.8134487813029264  1.2887474598448141 30.4707824317843432   T   T   T
  5.5128986757913667  1.2939408137831407 23.9322888437742805   T   T   T
  1.5836425983258575  5.3690422411920959 26.0668588650347850   T   T   T
  2.3777892895242485  3.9983620022836934 28.3528410437830161   T   T   T
  0.8057323090632773  4.0080086032439475 23.9320557377065342   T   T   T
  0.8154535291973812  3.9990715620364874 30.4709376440710002   T   T   T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Os E_tot= -271.85769952 eV
 D3-zero damping= -4.7586425 eV, D3-BJ damping= -6.9745807 eV
Al  O Al  O  H
 1.0000000000000000
     4.6911111462397965    0.0000000000000000    0.0000000000000000
    -2.3455555731198974    4.0626214246200014    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.8555449479953303
  11  18   1   3   6
Selective dynamics
Cartesian
  0.0230822744681551 -0.0584249134838246 12.3918657751636392   F   F   F
  2.3685569689828343  1.2994457670366362 16.7451569513452085   T   T   T
  0.0229182648088698 -0.0548557862726048 18.9527574136388743   T   T   T
  2.3707135835877091  1.2957287017431771 10.0985295441362890   F   F   F
  0.0229942841942676  2.6523878404961625 14.5561856244294301   F   F   F
  0.0558541388897946 -0.0447192065504144  9.7781175373791616   F   F   F
  2.3695404914643965  1.2987157322505378 14.0665571956713524   F   F   F
  0.0228304232237140  2.6550150475479648 18.4785176844579304   T   T   T
  0.0237171599104762 -0.0552747484533165 16.2873258757792101   T   T   T
  2.3762500941705911  1.2939466384703826 20.7726629259482927   T   T   T
  0.0285063672040412  2.6514121294813311 11.8834768182986377   F   F   F
  1.4798259548502117 -0.0543846453104392 11.0348070799988349   F   F   F
  3.8129087163956141  1.2963533085682162 15.4170027331878252   T   T   T
  1.4825556303773499  2.6434729919159117 19.8227930687438239   T   T   T
  0.7439280113174129  1.1962359887643237 17.6191421987870136   T   T   T
  3.0888712207647511  2.6000732724980651  8.8712015584813955   F   F   F
  0.7438888227654091  3.8971878577978849 13.2250185171475483   F   F   F
 -0.7050223729317278  1.1993254348321216 11.0371856277262967   F   F   F
  1.6487115283729499  2.5495985124876546 15.4170054273223460   T   T   T
 -0.7058707380180941  3.9100030182384993 19.8296193993697258   T   T   T
  3.2699443615923371 -0.0542752205609338 17.6201052488726795   T   T   T
  0.9156497881401405  1.2440906916107350  8.8494658732768272   F   F   F
 -1.4129572275389015  2.6540003637887635 13.2250148374957792   F   F   F
  1.6568471829279845  2.7522570334512015 11.0407582029264013   F   F   F
  1.6461877240142011  0.0497305230891644 15.4177315297506610   T   T   T
 -0.7113731933641289  1.4006766011101397 19.8268927573786158   T   T   T
 -1.5992179096564776  2.7579851163855986 17.6157938888463157   T   T   T
  3.1556708290406270 -0.0002981322266053  8.9135372731794220   F   F   F
  0.7426603942205980  1.4051106191437441 13.2221143204608840   F   F   F
  0.0264201811855569  2.6423494436698900 21.0978245382685969   T   T   T
  3.1268253767579237  2.6638089080490781 22.0140382446370353   T   T   T
  0.9546110484325694  1.3978016926829295 22.0293144510695846   T   T   T
  3.0643043409116442  0.0069435410150485 22.0077471530520619   T   T   T
  0.4101188344700492  2.0658167457023455  8.8276013437729759   F   F   F
  2.6162977243998191  2.4675066148228733  8.0391937587954807   F   F   F
  3.0940183027339434  0.3046998065084267  8.0000000000000000   F   F   F
  3.1072492984841915  2.1750261536430653 22.8555803765667598   T   T   T
  0.7653663968812656  0.4904952886564835 22.3257852423302730   T   T   T
  4.0091756016730180 -0.2424629368417825 22.0482971047804313   T   T   T

Oxidized reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Os E_tot= -252.40231159
eV
 D3-zero damping= -4.475416 eV, D3-BJ damping= -6.6631924 eV
Al  O Al  O  H
 1.0000000000000000
     4.6911111462397965    0.0000000000000000    0.0000000000000000
```

```
    -2.3455555731198974    4.0626214246200014    0.0000000000000000
     0.0000000000000018    0.0000000000000032   29.8754197198952873
  11  18   1   3   3
Selective dynamics
Cartesian
  0.0230822744681551 -0.0584249134838246 12.3918657751636392   F   F   F
  2.3693760186115473  1.2972652223758638 16.7428714541413264   T   T   T
  0.0241247425651116 -0.0559972562239924 18.9476000072428583   T   T   T
  2.3707135835877091  1.2957287017431771 10.0985295441362890   F   F   F
  0.0229942841942676  2.6523878404961625 14.5561856244294301   F   F   F
  0.0558541388897946 -0.0447192065504144  9.7781175373791616   F   F   F
  2.3695404914643965  1.2987157322505378 14.0665571956713524   F   F   F
  0.0238028457302801  2.6520470938375893 18.4774762936457506   T   T   T
  0.0236646423981811 -0.0565636413949494 16.2837023692268232   T   T   T
  2.3697052496188724  1.2995162611371405 20.7672376821084228   T   T   T
  0.0285063672040412  2.6514121294813311 11.8834768182986377   F   F   F
  1.4798259548502117 -0.0543846453104392 11.0348070799988349   F   F   F
  3.8129645374305841  1.2970813121919598 15.4220498141685614   T   T   T
  1.4821676867872997  2.6661978855377813 19.8347343350881680   T   T   T
  0.7472247496809507  1.1953588620986157 17.6217124924651998   T   T   T
  3.0888712207647511  2.6000732724980651  8.8712015584813955   F   F   F
  0.7438888227654091  3.8971878577978849 13.2250185171475483   F   F   F
 -0.7050223729317278  1.1993254348321216 11.0371856277262967   F   F   F
  1.6479851078421028  2.5480949800411601 15.4217827509366519   T   T   T
 -0.7162567198112858  3.9092136673057540 19.8348205008391076   T   T   T
  3.2692533334428449 -0.0557786066363294 17.6221764674093748   T   T   T
  0.9156497881401405  1.2440906916107350  8.8494658732768272   F   F   F
 -1.4129572275389015  2.6540003637887635 13.2250148374957792   F   F   F
  1.6568471829279845  2.7522570334512015 11.0407582029264013   F   F   F
  1.6468888763404086  0.0482468689997851 15.4224060592826060   T   T   T
 -0.6932491867995819  1.3836320143464464 19.8349083596760423   T   T   T
 -1.5993586385084744  2.7536917165537744 17.6217125574379985   T   T   T
  3.1556708290406270 -0.0002981322266053  8.9135372731794220   F   F   F
  0.7426603942205980  1.4051106191437441 13.2221143204608840   F   F   F
  0.0243782737443591  2.6538094664858098 21.1074380154606871   T   T   T
  3.3101204950268706  2.1727729102588227 22.2083391934307137   T   T   T
  1.1450171991578189  1.6795838534487149 22.2090686592688620   T   T   T
  2.6557187455020812  0.0498875455647122 22.2080267077780533   T   T   T
  0.4101188344700492  2.0658167457023455  8.8276013437729759   F   F   F
  2.6162977243998191  2.4675066148228733  8.0391937587954807   F   F   F
  3.0940183027339434  0.3046998065084267  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Os E_tot= -131.66202437 eV
 D3-zero damping= -4.9347895 eV, D3-BJ damping= -5.6826056 eV
Os
 1.0000000000000000
     4.6911111462397965    0.0000000000000000    0.0000000000000000
     2.3455555731198983    4.0626214246199996    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.5181175745043944
  12
Cartesian
  5.4729713275382945  1.3542633401464219 10.1234824116889346
  5.4729712915703885  4.0626775841355238 10.1234824332284923
  4.6911718731439196  2.7084053483967452 14.5181175240911422
  2.3455395212486621  1.3541817919957424  8.0000000644248210
  3.1274157730324705  2.7084705052898488 10.1234824187008581
  1.5637178571295671  2.7083198732010878 12.3946422896051978
  2.3456162758842845  1.3541982087791373 14.5181175745043980
  4.6910950931724695 -0.0000253472406302  8.0000000000000000
  2.3456163511148400  4.0626124902989318 14.5181174973710174
  3.9092735477788745  1.3541127452899817 12.3946423073664356
  4.6910950253257564  2.7083889149862732  8.0000001299296297
  3.9092735372334895  4.0625270047634157 12.3946422904132660
```

```
Interface: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ru E_tot= -369.79135647 eV
 D3-zero damping= -10.7224361 eV, D3-BJ damping= -13.7851476 eV
Al  O Al  O  H Ru
 1.0000000000000000
     4.6179847559130716    0.0000000000000000    0.0000000000000000
    -2.3089923779565349    3.9992921129100010    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.4024068536711241
  11  18   1   3   3  12
Selective dynamics
Cartesian
  0.0227224613322544 -0.0575141691217670 12.3918657751636410   F   F   F
  2.3328025035918096  1.2762207500407095 16.7473458706000500   T   T   T
  0.0247035751592593 -0.0585911557629503 18.9841909702427500   T   T   T
  2.3337582181184291  1.2755305099188028 10.0985295441362908   F   F   F
  0.0226358426760739  2.6110416556637159 14.5561856244294319   F   F   F
  0.0549834685018009 -0.0440221106915946  9.7781175373791633   F   F   F
  2.3326034124926704  1.2784709777351528 14.0665571956713542   F   F   F
  0.0243604356073304  2.6085590749138241 18.5047740515187868   T   T   T
  0.0235040417490847 -0.0563747246988023 16.3158107101638201   T   T   T
  2.3344291638428887  1.2733707911560230 20.8414419527644199   T   T   T
  0.0280620017498928  2.6100811543129261 11.8834768182986394   F   F   F
  1.4567580020738775 -0.0535368818111797 11.0348070799988367   F   F   F
  3.7571820055708574  1.2739926100812449 15.4258647079398585   T   T   T
  1.4620965044751009  2.5914804798433693 19.8564391542020893   T   T   T
  0.7367405902280993  1.1758369189003222 17.6398761415918592   T   T   T
  3.0407210074107818  2.5595425822041071  8.8712015584813972   F   F   F
  0.7322928697561025  3.8364373721279099 13.2250185171475501   F   F   F
 -0.6940322813255196  1.1806300048705864 11.0371856277262985   F   F   F
  1.6227810161147969  2.5127161599158705 15.4254749389468593   T   T   T
 -0.6803543313805460  3.8594952715175661 19.8567510790329962   T   T   T
  3.2174429770715247 -0.0562362645527502 17.6399776532982031   T   T   T
  0.9013763757815803  1.2246974479461730  8.8494658732768290   F   F   F
 -1.3909316437241166  2.6126290424792584 13.2250148374957810   F   F   F
  1.6310197723138398  2.7093540589034868 11.0407582029264031   F   F   F
  1.6170937112695687  0.0456914763761645 15.4260691869350666   T   T   T
 -0.7074844047662366  1.3705266756075680 19.8562246806327316   T   T   T
 -1.5735683769809428  2.7080590768211388 17.6399672115591351   T   T   T
  3.1064793241725202 -0.0002934848556750  8.9135372731794238   F   F   F
  0.7310835903089052  1.3832073505183369 13.2221143204608858   F   F   F
  0.0257459767887237  2.6056903176756574 21.0968142507638241   T   T   T
  3.1038756606726357  2.5236144434492380 22.0646269193727669   T   T   T
  0.8666348993692152  1.3112004589598285 22.0638858558165616   T   T   T
  3.0355822587849746 -0.0192502393673975 22.0635176888748852   T   T   T
  0.4037257840743370  2.0336141998703621  8.8276013437729777   F   F   F
  2.5755141226813354  2.4290424117323228  8.0391937587954825   F   F   F
  3.0457878551852620  0.2999500582529259  8.0000000000000018   F   F   F
 -0.7201724341915753  3.9369990460609867 26.0703029020114379   T   T   T
  0.0287836658168447  2.5980628960536118 28.3132000057757374   T   T   T
  3.1004526527728360  2.5940318057592555 23.9671934218758409   T   T   T
  1.5562152503400648  2.5795962207483996 26.0684155449057826   T   T   T
  2.3376382658758934  1.2647519310266122 28.3138372799472968   T   T   T
  3.1083912224531245  2.5955206376588116 30.4016988982930947   T   T   T
  0.8007463249461307  1.2587344108093075 30.4018204086911830   T   T   T
  5.4235643297882756  1.2667846767294773 23.9663576437113264   T   T   T
  1.5521052106639763  5.2850855814663076 26.0695620701716564   T   T   T
  2.3381659693747179  3.9309878722291298 28.3266531050674608   T   T   T
  0.7939827187101610  3.9431711748248319 23.9658063100830354   T   T   T
  0.8032812175167147  3.9271700023141043 30.4017334678803515   T   T   T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ru E_tot= -270.68097316 eV
 D3-zero damping= -4.893999 eV, D3-BJ damping= -7.1775556 eV
Al  O Al  O  H
```

```
 1.0000000000000000
     4.6179847559130716    0.0000000000000000    0.0000000000000000
    -2.3089923779565349    3.9992921129100010    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.9035805297168196
  11  18   1   3   6
Selective dynamics
Cartesian
  0.0227224613322544 -0.0575141691217670 12.3918657751636392   F   F   F
  2.3308498112092515  1.2792505470692801 16.7508252320481255   T   T   T
  0.0211333403753524 -0.0531083389474550 18.9763103955494437   T   T   T
  2.3337582181184291  1.2755305099188028 10.0985295441362890   F   F   F
  0.0226358426760739  2.6110416556637159 14.5561856244294301   F   F   F
  0.0549834685018009 -0.0440221106915946  9.7781175373791616   F   F   F
  2.3326034124926704  1.2784709777351528 14.0665571956713524   F   F   F
  0.0213132629345229  2.6142782051927966 18.5249684935048968   T   T   T
  0.0227665684053965 -0.0543907837117405 16.3168658574007175   T   T   T
  2.3380698518339207  1.2751442151095396 20.8253034776699764   T   T   T
  0.0280620017498928  2.6100811543129261 11.8834768182986377   F   F   F
  1.4567580020738773 -0.0535368818111797 11.0348070799988349   F   F   F
  3.7562603567148973  1.2750042986405716 15.4266825214809344   T   T   T
  1.4618634393870953  2.6029606756343107 19.8648330860017381   T   T   T
  0.7340336401898094  1.1820031309547039 17.6455522237794824   T   T   T
  3.0407210074107818  2.5595425822041071  8.8712015584813955   F   F   F
  0.7322928697561025  3.8364373721279099 13.2250185171475483   F   F   F
 -0.6940322813255195  1.1806300048705864 11.0371856277262967   F   F   F
  1.6219423908385573  2.5140973688763997 15.4266948948026350   T   T   T
 -0.6976626522800712  3.8541899463007927 19.8719158883802116   T   T   T
  3.2133542442662422 -0.0524713528566282 17.6468972751140427   T   T   T
  0.9013763757815803  1.2246974479461727  8.8494658732768272   F   F   F
 -1.3909316437241166  2.6126290424792584 13.2250148374957792   F   F   F
  1.6310197723138398  2.7093540589034868 11.0407582029264013   F   F   F
  1.6168973786218774  0.0469414185664441 15.4270946805265865   T   T   T
 -0.7036945738629823  1.3774855273004187 19.8670172392453992   T   T   T
 -1.5734761975660190  2.7113891670268000 17.6426473830957278   T   T   T
  3.1064793241725202 -0.0002934848556750  8.9135372731794220   F   F   F
  0.7310835903089052  1.3832073505183369 13.2221143204608840   F   F   F
  0.0253477376688938  2.6027146384646613 21.1435078693575136   T   T   T
  3.0709284500622140  2.6381460004769428 22.0755275780057225   T   T   T
  0.9317466923010155  1.3714545222871108 22.0909127230871540   T   T   T
  3.0271846343306734  0.0141427323397033 22.0649771178203338   T   T   T
  0.4037257840743370  2.0336141998703621  8.8276013437729759   F   F   F
  2.5755141226813354  2.4290424117323228  8.0391937587954807   F   F   F
  3.0457878551852620  0.2999500582529259  8.0000000000000000   F   F   F
  3.0565885102735044  2.1266906275678759 22.9036109565470092   T   T   T
  0.7661819667946494  0.4594601099488254 22.3877902280914896   T   T   T
  3.9672308881886762 -0.2550887167857658 22.1074204751087002   T   T   T

Oxidized reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ru E_tot= -251.42626608
eV
 D3-zero damping= -4.609496 eV, D3-BJ damping= -6.8596881 eV
Al  O Al  O  H
 1.0000000000000000
     4.6179847559130716    0.0000000000000000    0.0000000000000000
    -2.3089923779565349    3.9992921129100010    0.0000000000000000
     0.0000000000000018    0.0000000000000032   29.8754197198952873
  11  18   1   3   3
Selective dynamics
Cartesian
  0.0227224613322544 -0.0575141691217670 12.3918657751636392   F   F   F
  2.3324938915007731  1.2783415914505887 16.7480226614959982   T   T   T
  0.0237108951154689 -0.0542214670019601 18.9714175766668696   T   T   T
  2.3337582181184291  1.2755305099188028 10.0985295441362890   F   F   F
  0.0226358426760739  2.6110416556637159 14.5561856244294301   F   F   F
```

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  0.0549834685018009 -0.0440221106915946  9.7781175373791616   F   F   F
  2.3326034124926704  1.2784709777351528 14.0665571956713524   F   F   F
  0.0241861076958680  2.6118763349385987 18.5240608081031617   T   T   T
  0.0235386777397822 -0.0549057001753989 16.3140067931782831   T   T   T
  2.3328431011035495  1.2794865686627375 20.8214267192385023   T   T   T
  0.0280620017498928  2.6100811543129261 11.8834768182986377   F   F   F
  1.4567580020738773 -0.0535368818111797 11.0348070799988349   F   F   F
  3.7569649042593376  1.2758311798408963 15.4318377339768595   T   T   T
  1.4627431413828207  2.6230792191894512 19.8761473977234608   T   T   T
  0.7378217704356279  1.1815577600735230 17.6476508494112565   T   T   T
  3.0407210074107818  2.5595425822041071  8.8712015584813955   F   F   F
  0.7322928697561025  3.8364373721279099 13.2250185171475483   F   F   F
 -0.6940322813255195  1.1806300048705864 11.0371856277262967   F   F   F
  1.6217698212283227  2.5130542576993200 15.4317718240756001   T   T   T
 -0.7056408320611950  3.8538077362442471 19.8763277253550790   T   T   T
  3.2139576100733445 -0.0532510293168918 17.6482156708530731   T   T   T
  0.9013763757815803  1.2246974479461727  8.8494658732768272   F   F   F
 -1.3909316437241166  2.6126290424792584 13.2250148374957792   F   F   F
  1.6310197723138398  2.7093540589034868 11.0407582029264013   F   F   F
  1.6180484054016844  0.0457627114821737 15.4321331003086559   T   T   T
 -0.6859458723427304  1.3598964483797313 19.8785678716413408   T   T   T
 -1.5720550034105818  2.7076217414041057 17.6479651172515304   T   T   T
  3.1064793241725202 -0.0002934848556750  8.9135372731794220   F   F   F
  0.7310835903089052  1.3832073505183369 13.2221143204608840   F   F   F
  0.0226195247637993  2.6135864795789465 21.1489633311651524   T   T   T
  3.2421825113921576  2.1735168697579188 22.2637535679085765   T   T   T
  1.1115732992648648  1.6355072875420742 22.2657822985346279   T   T   T
  2.6413421464591851  0.0451668358554329 22.2638908730457565   T   T   T
  0.4037257840743370  2.0336141998703621  8.8276013437729759   F   F   F
  2.5755141226813354  2.4290424117323228  8.0391937587954807   F   F   F
  3.0457878551852620  0.2999500582529259  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt3/Ru E_tot= -108.70923104 eV
 D3-zero damping= -4.7429262 eV, D3-BJ damping= -5.6232816 eV
Ru
 1.0000000000000000
     4.6179847559130716    0.0000000000000000    0.0000000000000000
     2.3089923779565358    3.9992921129099992    0.0000000000000000
     0.0000000000000000    0.0000000000000000   22.4084815249538565
  12
Cartesian
  5.3877199732719454  1.3330671769786648 10.0948982599007611
  5.3876921316083086  3.9992800040548420 10.0948848681609267
  4.6180363988259918  2.6661662101717183 14.4091451294994801
  2.3089084437188805  1.3330701002028027  7.9992881352323799
  3.0786258182463726  2.6662217864006115 10.0949228697323594
  1.5393391741777305  2.6661811884859241 12.3135791330974556
  2.3090901342500652  1.3330785067888125 14.4091996535252846
  4.6179610423846977 -0.0000268395427653  7.9992451285714274
  2.3090480515514482  3.9992383029447227 14.4091666204827256
  3.8483377229941835  1.3330847420037120 12.3135932515719038
  4.6179538097811115  2.6661963023548161  7.9992814524803357
  3.8483403818493844  3.9992736049538200 12.3135768863677395

Interface: ZnO(10-10)/fcc(100)_5x2/Au E_tot= -384.44310703 eV
 D3-zero damping= -27.3979517 eV, D3-BJ damping= -26.0458459 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Au
 1.0000000000000000
    14.4937585523500019    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7975034209400009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.1824709295180504
```

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   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2  30
Selective dynamics
Cartesian
  3.6233506493801433  5.7920814396558580  8.9451241821253618   F   F   F
  1.8116330556198461  2.8933297495539323  8.0000001838787966   F   F   F
  3.6233512433442532  3.5940765006679847  8.9451248436730744   F   F   F
  1.8116320522632581  0.6953248071507115  8.0000000000000000   F   F   F
  1.8116359099072228  5.7920813601461925 11.7805090714841079   F   F   F
  3.6233579542344261  2.8933296700442663 10.8353850732375427   F   F   F
  1.8116365038713327  3.5940764211583196 11.7805097330318205   F   F   F
  3.6233569508778385  0.6953247276410457 10.8353848893587461   F   F   F
  3.6130098061835603  5.6650358001966312 14.2857236745722478   T   T   T
  1.8071121390916134  2.8455519522919701 13.6207565964986976   T   T   T
  3.6294838892061492  3.5947599420337699 14.3056957935194262   T   T   T
  1.8068535303797739  0.6923978193031749 13.6557179133581137   T   T   T
  1.7963601428808977  5.7377099749585030 16.7442911382059343   T   T   T
  3.6414649897855291  2.8551479382308060 16.2126371046256708   T   T   T
  1.8444221488920545  3.7431035792440444 16.6982111899142005   T   T   T
  3.6291461843282438  0.7559472119087169 16.1600387725862937   T   T   T
  7.2467902874676433  5.7920814396558580  8.9451241821253618   F   F   F
  5.4350726937073475  2.8933297495539323  8.0000001838787966   F   F   F
  7.2467908814317541  3.5940765006679847  8.9451248436730744   F   F   F
  5.4350716903507585  0.6953248071507115  8.0000000000000000   F   F   F
  5.4350755479947228  5.7920813601461925 11.7805090714841079   F   F   F
  7.2467975923219266  2.8933296700442663 10.8353850732375427   F   F   F
  5.4350761419588327  3.5940764211583196 11.7805097330318205   F   F   F
  7.2467965889653385  0.6953247276410457 10.8353848893587461   F   F   F
  7.2468097889917820  5.6539305255396357 14.2813182696273326   T   T   T
  5.4327947109165136  2.8283186266731279 13.6060179424895527   T   T   T
  7.2469077638434607  3.5857576208053086 14.2905017161737842   T   T   T
  5.4309181103949902  0.6846065903440863 13.6560505963593535   T   T   T
  5.4188886361425821  5.7316561454656911 16.6880042042995527   T   T   T
  7.2468504906429470  2.8171631523999290 16.1859383568511461   T   T   T
  5.4565104323422435  3.7144001978771009 16.6703204751771672   T   T   T
  7.2468998656554344  0.7395130236613623 16.1522069502572876   T   T   T
 10.8702299255551438  5.7920814396558580  8.9451241821253618   F   F   F
  9.0585123317948462  2.8933297495539323  8.0000001838787966   F   F   F
 10.8702305195192537  3.5940765006679847  8.9451248436730744   F   F   F
  9.0585113284382590  0.6953248071507115  8.0000000000000000   F   F   F
  9.0585151860822251  5.7920813601461925 11.7805090714841079   F   F   F
 10.8702372304094279  2.8933296700442663 10.8353850732375427   F   F   F
  9.0585157800463332  3.5940764211583196 11.7805097330318205   F   F   F
 10.8702362270528408  0.6953247276410457 10.8353848893587461   F   F   F
 10.8805451741892796  5.6649749947927077 14.2854803081158845   T   T   T
  9.0610767515623465  2.8283116652260580 13.6059503283549859   T   T   T
 10.8642185434932195  3.5947694522545253 14.3054658602818918   T   T   T
  9.0625746772234628  0.6845432237302082 13.6560215192117074   T   T   T
  9.0750677200001206  5.7317317835930028 16.6875436454203054   T   T   T
 10.8522655989820009  2.8552780951015624 16.2124312771322465   T   T   T
  9.0373216229848747  3.7144745533297114 16.6701011026974761   T   T   T
 10.8646909582210007  0.7561062073669398 16.1595939602461591   T   T   T
 14.4936695636426460  5.7920814396558580  8.9451241821253618   F   F   F
 12.6819519698823484  2.8933297495539323  8.0000001838787966   F   F   F
 14.4936701576067577  3.5940765006679847  8.9451248436730744   F   F   F
 12.6819509665257595  0.6953248071507115  8.0000000000000000   F   F   F
 12.6819548241697273  5.7920813601461925 11.7805090714841079   F   F   F
 14.4936768684969284  2.8933296700442663 10.8353850732375427   F   F   F
 12.6819554181338354  3.5940764211583196 11.7805097330318205   F   F   F
 14.4936758651403430  0.6953247276410457 10.8353848893587461   F   F   F
 14.4937840701344509  5.6796758158504170 14.2968099670604900   T   T   T
 12.6866414836972154  2.8454973587845229 13.6208626364462706   T   T   T
 14.4937783993535181  3.6021357492038426 14.3394894887300453   T   T   T
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 12.6869259212716781  0.6924174285660581 13.6557482625972675   T   T   T
 12.6974132201833854  5.7375259862127646 16.7438656823657936   T   T   T
 14.4937237782525035  2.8960082822553450 16.2625600885459534   T   T   T
 12.6492404304496038  3.7430619964406708 16.6979888603448998   T   T   T
 14.4938590555803923  0.7682990685796020 16.1817206270766007   T   T   T
 -0.0001044675263884  1.0671838902223325 18.9897226397177725   T   T   T
  1.4445034740776357  2.4832715373158791 21.0750005541141050   T   T   T
  0.0002356962972012  1.0343536278982381 23.1773521728667831   T   T   T
 -0.0000193450837716  3.9605122554011962 19.0236550690827357   T   T   T
  1.4525812785323369  5.3938212700414256 21.0637750846844725   T   T   T
  0.0000995812885428  3.9429700630322468 23.1408024018725804   T   T   T
  2.9125396780072919  1.0414131300282357 18.9734980084204636   T   T   T
  4.3252755007275860  2.4992184909399957 21.0594134201935148   T   T   T
  2.9110826561360135  1.0328843705457151 23.1498061280682315   T   T   T
  2.8711529204900166  3.9123051765002557 18.9623717926994821   T   T   T
  4.3377758194713945  5.3503169414883738 21.0287981123243917   T   T   T
  2.8896431343869979  3.9400805538650614 23.1616108034035975   T   T   T
  5.8076413563057248  1.0785903601700526 19.0175141936035992   T   T   T
  7.2470872668788990  2.5170173539567933 21.0680722333979595   T   T   T
  5.8022807516714572  1.0137181265205304 23.0816940856945969   T   T   T
  5.7786150970986050  3.9263893486858037 18.9474231703520992   T   T   T
  7.2467904834394883  5.3356615615928256 21.0163475061752578   T   T   T
  5.7888241745545024  3.9224387078488578 23.1755664948676205   T   T   T
  8.6858775234475196  1.0785688069842294 19.0171542539126754   T   T   T
 10.1685141332199489  2.4996511787372842 21.0588470050216472   T   T   T
  8.6928959904943621  1.0144405586758489 23.0815512879055156   T   T   T
  8.7145318688135074  3.9263957394738029 18.9472187054301209   T   T   T
 10.1562005126352304  5.3504485111201179 21.0283934292643799   T   T   T
  8.7059727826875353  3.9233175874768471 23.1751288576560839   T   T   T
 11.5811845826094029  1.0409534167071419 18.9731726863670644   T   T   T
 13.0493926410427736  2.4834499037703002 21.0748409573143007   T   T   T
 11.5835067651926611  1.0337094049312792 23.1492689573543196   T   T   T
 11.6222410184014482  3.9119933807951299 18.9620172472672550   T   T   T
 13.0413848054002184  5.3940823598277046 21.0635396038579792   T   T   T
 11.6046085862685668  3.9407313778068298 23.1618495748901942   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_5x2/Au E_tot= -276.5835402 eV
 D3-zero damping= -9.6614711 eV, D3-BJ damping= -9.8632005 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O
 1.0000000000000000
    14.4937585523500019    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7975034209400009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.9371186129033156
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.6233506493801433  5.7920814396558580  8.9451241821253618   F   F   F
  1.8116330556198461  2.8933297495539323  8.0000001838787966   F   F   F
  3.6233512433442532  3.5940765006679847  8.9451248436730744   F   F   F
  1.8116320522632581  0.6953248071507115  8.0000000000000000   F   F   F
  1.8116359099072228  5.7920813601461925 11.7805090714841079   F   F   F
  3.6233579542344261  2.8933296700442663 10.8353850732375427   F   F   F
  1.8116365038713327  3.5940764211583196 11.7805097330318205   F   F   F
  3.6233569508778385  0.6953247276410457 10.8353848893587461   F   F   F
  3.6234523177753339  5.6816202269352818 14.2833334692896425   T   T   T
  1.8115550108091483  2.8760124806469349 13.6371222901510034   T   T   T
  3.6234311633775458  3.6000636545689679 14.2925785984796150   T   T   T
  1.8116777521490985  0.6947644265135325 13.6547659480132744   T   T   T
  1.8116926211349342  5.5016671449481551 16.5379714712193753   T   T   T
  3.6234721234528924  2.8115074251033696 16.2428926848938247   T   T   T
  1.8119502096625797  3.5746913636139768 16.7124684248461008   T   T   T
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  3.6234512578108897  0.6292990545291974 16.2426386830899965   T   T   T
  7.2467902874676433  5.7920814396558580  8.9451241821253618   F   F   F
  5.4350726937073475  2.8933297495539323  8.0000001838787966   F   F   F
  7.2467908814317541  3.5940765006679847  8.9451248436730744   F   F   F
  5.4350716903507585  0.6953248071507115  8.0000000000000000   F   F   F
  5.4350755479947228  5.7920813601461925 11.7805090714841079   F   F   F
  7.2467975923219266  2.8933296700442663 10.8353850732375427   F   F   F
  5.4350761419588327  3.5940764211583196 11.7805097330318205   F   F   F
  7.2467965889653385  0.6953247276410457 10.8353848893587461   F   F   F
  7.2468728938257891  5.6818294235403917 14.2836110667743146   T   T   T
  5.4352916362948305  2.8759826151295904 13.6371044920020044   T   T   T
  7.2468589283410534  3.6000594095320926 14.2926773969450540   T   T   T
  5.4351539609627153  0.6947696976890994 13.6547550836288281   T   T   T
  5.4352178117255567  5.5016630485542981 16.5379752919261271   T   T   T
  7.2468879258690260  2.8115766237983140 16.2431250058322689   T   T   T
  5.4349373890143777  3.5747288677944948 16.7125031466354272   T   T   T
  7.2469143362474533  0.6292130902780133 16.2430156553274259   T   T   T
 10.8702299255551438  5.7920814396558580  8.9451241821253618   F   F   F
  9.0585123317948462  2.8933297495539323  8.0000001838787966   F   F   F
 10.8702305195192537  3.5940765006679847  8.9451248436730744   F   F   F
  9.0585113284382590  0.6953248071507115  8.0000000000000000   F   F   F
  9.0585151860822251  5.7920813601461925 11.7805090714841079   F   F   F
 10.8702372304094279  2.8933296700442663 10.8353850732375427   F   F   F
  9.0585157800463332  3.5940764211583196 11.7805097330318205   F   F   F
 10.8702362270528408  0.6953247276410457 10.8353848893587461   F   F   F
 10.8703309646044701  5.6816208430582256 14.2833326709146924   T   T   T
  9.0584218472569003  2.8760161034377449 13.6371305551686550   T   T   T
 10.8703080887626289  3.6000641962758149 14.2925809744486738   T   T   T
  9.0585576030495325  0.6947640756048733 13.6547670065591475   T   T   T
  9.0585687189275710  5.5016689197617481 16.5379687292033566   T   T   T
 10.8703560474876539  2.8115112355344425 16.2428939201517437   T   T   T
  9.0588258852446657  3.5746915087710756 16.7124721247585164   T   T   T
 10.8703302951627645  0.6292962382177237 16.2426392336554137   T   T   T
 14.4936695636426460  5.7920814396558580  8.9451241821253618   F   F   F
 12.6819519698823484  2.8933297495539323  8.0000001838787966   F   F   F
 14.4936701576067577  3.5940765006679847  8.9451248436730744   F   F   F
 12.6819509665257595  0.6953248071507115  8.0000000000000000   F   F   F
 12.6819548241697273  5.7920813601461925 11.7805090714841079   F   F   F
 14.4936768684969284  2.8933296700442663 10.8353850732375427   F   F   F
 12.6819554181338354  3.5940764211583196 11.7805097330318205   F   F   F
 14.4936758651403430  0.6953247276410457 10.8353848893587461   F   F   F
 14.4937529023779419  5.6818305597688896 14.2836091198110342   T   T   T
 12.6821643646866598  2.8759817954782938 13.6371017106237549   T   T   T
 14.4937427013893494  3.6000600591899974 14.2926545498050697   T   T   T
 12.6820342567649469  0.6947698097735271 13.6547555638161402   T   T   T
 12.6820998708810588  5.5016521371416811 16.5379744215944875   T   T   T
 14.4937573757161431  2.8115936430547972 16.2430576968312579   T   T   T
 12.6818303268250165  3.5747176766551614 16.7124827337562394   T   T   T
 14.4937976103673840  0.6292102647436029 16.2430066965056454   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_5x2/Au E_tot= -100.02593061 eV
 D3-zero damping= -12.2942905 eV, D3-BJ damping= -12.3918889 eV
Au
 1.0000000000000000
    14.4937585523500019    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7975034209400009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.8120708806377266
  30
Cartesian
  0.0000135913506753  0.0000002224711026  7.8115425234445661
  1.4472671591766977  1.4493760135937048  9.9059877087538499
  0.0000084975706455 -0.0000000777413756 12.0004594716362991
  0.0000134016638376  2.8987514597414550  7.8115434866012254
```

```
  1.4472677430941705  4.3481273287092153  9.9059873345378051
  0.0000082658355334  2.8987514422378275 12.0004572559455340
  2.8947911112705991  0.0000007400953112  7.8168612580265906
  4.3476271929633432  1.4493757882025793  9.9060720324687548
  2.8947907614409125  0.0000007348703053 11.9951716875696821
  2.8947908624419849  2.8987509360170982  7.8168618599631410
  4.3476257965253966  4.3481275356967517  9.9060720940677882
  2.8947904655437804  2.8987509694995359 11.9951711916334993
  5.7984762629680153 -0.0000004168108664  7.8154246160690812
  7.2468555421086176  1.4493759395753456  9.9059511638366118
  5.7985565393236591 -0.0000002698571941 11.9965907290318601
  5.7984761215201477  2.8987520929232704  7.8154242830103202
  7.2468546926103148  4.3481275987589614  9.9059517498837018
  5.7985565236182239  2.8987520357074228 11.9965906932916830
  8.6951919013823868 -0.0000010586332160  7.8156619863133105
 10.1461554606336648  1.4493758833140435  9.9060541688682715
  8.6952168317763103 -0.0000006805728984 11.9965712767816282
  8.6951916814240189  2.8987525479087290  7.8156616865917066
 10.1461562252179789  4.3481276273637839  9.9060546182273654
  8.6952173117810663  2.8987527963029311 11.9965710819532934
 11.5989821374130067 -0.0000003346905815  7.8168499519234143
 13.0465177432936308  1.4493760332743522  9.9059742229750292
 11.5989800101073222 -0.0000004115494857 11.9951318491821901
 11.5989818767664179  2.8987520795181743  7.8168529103120798
 13.0465187867960992  4.3481273423265385  9.9059741342465273
 11.5989803310301340  2.8987522859393859 11.9951291754853386

Interface: ZnO(10-10)/fcc(100)_5x2/Ag E_tot= -367.49266384 eV
 D3-zero damping= -23.7305123 eV, D3-BJ damping= -24.9139342 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Ag
 1.0000000000000000
    14.4026352597500011    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7610541039000012    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.1824709295180504
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2  30
Selective dynamics
Cartesian
  3.6005703857084863  5.7556662109984709  8.9451241821253618   F   F   F
  1.8002431895326734  2.8751391792884893  8.0000001838787966   F   F   F
  3.6005709759383016  3.5714802856548644  8.9451248436730744   F   F   F
  1.8002421924842598  0.6909532505510081  8.0000000000000000   F   F   F
  1.8002460258749422  5.7556661319886882 11.7805090714841079   F   F   F
  3.6005776446366298  2.8751391002787066 10.8353850732375427   F   F   F
  1.8002466161047572  3.5714802066450821 11.7805097330318205   F   F   F
  3.6005766475882166  0.6909531715412253 10.8353848893587461   F   F   F
  3.5950734492047420  5.6253518304037753 14.2969658880093977   T   T   T
  1.8016017148204659  2.8144572820572651 13.6146154227727383   T   T   T
  3.6013489120023729  3.5597329340317518 14.3278751732156326   T   T   T
  1.7968375021054930  0.6810119788520568 13.6655202305744368   T   T   T
  1.7758912277654610  5.6190294161025056 16.7339913539458855   T   T   T
  3.6145542096513221  2.7922634064554450 16.2172376058527803   T   T   T
  1.8135216817436692  3.6324522931193028 16.7819953936945865   T   T   T
  3.5925893098750783  0.6977949665103205 16.2183036458392387   T   T   T
  7.2012292006459866  5.7556662109984709  8.9451241821253618   F   F   F
  5.4009020044701739  2.8751391792884893  8.0000001838787966   F   F   F
  7.2012297908758027  3.5714802856548644  8.9451248436730744   F   F   F
  5.4009010074217603  0.6909532505510081  8.0000000000000000   F   F   F
  5.4009048408124416  5.7556661319886882 11.7805090714841079   F   F   F
  7.2012364595741305  2.8751391002787066 10.8353850732375427   F   F   F
  5.4009054310422568  3.5714802066450821 11.7805097330318205   F   F   F
  7.2012354625257160  0.6909531715412253 10.8353848893587461   F   F   F
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7.2011900076869360	5.6146089863677515	14.3116218572222831	T	T	T
5.4054850093406444	2.8102559772752436	13.6119110549499176	T	T	T
7.2011884244051210	3.5511663062124974	14.3263531740264742	T	T	T
5.4003888556337785	0.6748672397488212	13.6715508213245389	T	T	T
5.3733529220194596	5.6004748362164225	16.7025033403045633	T	T	T
7.2011345894603647	2.7687479922500478	16.2237243575499406	T	T	T
5.4117610660416995	3.6075247844599732	16.7362062593454759	T	T	T
7.2012198969117298	0.6799692548626528	16.2309642577154172	T	T	T
10.8018880155834864	5.7556662109984709	8.9451241821253618	F	F	F
9.0015608194076737	2.8751391792884893	8.0000001838787966	F	F	F
10.8018886058133017	3.5714802856548644	8.9451248436730744	F	F	F
9.0015598223592601	0.6909532505510081	8.0000000000000000	F	F	F
9.0015636557499441	5.7556661319886882	11.7805090714841079	F	F	F
10.8018952745116312	2.8751391002787066	10.8353850732375427	F	F	F
9.0015642459797576	3.5714802066450821	11.7805097330318205	F	F	F
10.8018942774632194	0.6909531715412253	10.8353848893587461	F	F	F
10.8075145603008131	5.6254553828240637	14.2968491978799843	T	T	T
8.9967846643297023	2.8104930280598164	13.6118745132431176	T	T	T
10.8010915727010826	3.5597278301883883	14.3276319243882373	T	T	T
9.0021226910781404	0.6748265337600530	13.6715364917048472	T	T	T
9.0289051606129398	5.6004826595012362	16.7018733851431449	T	T	T
10.7880847874843102	2.7921168591386909	16.2171262099393836	T	T	T
8.9909127221030989	3.6073090852089855	16.7358297785455719	T	T	T
10.8101043883272379	0.6976833101237359	16.2183066789836978	T	T	T
14.4025468305209881	5.7556662109984709	8.9451241821253618	F	F	F
12.6022196343451753	2.8751391792884893	8.0000001838787966	F	F	F
14.4025474207508051	3.5714802856548644	8.9451248436730744	F	F	F
12.6022186372967617	0.6909532505510081	8.0000000000000000	F	F	F
12.6022224706874457	5.7556661319886882	11.7805090714841079	F	F	F
14.4025540894491328	2.8751391002787066	10.8353850732375427	F	F	F
12.6022230609172592	3.5714802066450821	11.7805097330318205	F	F	F
14.4025530924007192	0.6909531715412253	10.8353848893587461	F	F	F
14.4026071418378052	5.6278631984343894	14.2903721790509426	T	T	T
12.6008193091810341	2.8144130703107124	13.6145622271614215	T	T	T
14.4026248555599086	3.5629761120739394	14.3379667411654577	T	T	T
12.6057332589421414	0.6810229669008478	13.6655911366800495	T	T	T
12.6269398628327956	5.6187308172997064	16.7336893027686635	T	T	T
14.4026053456114624	2.8160925492879088	16.2278219784165181	T	T	T
12.5890415177471748	3.6322668301953578	16.7812972236520004	T	T	T
14.4027676697345832	0.7137393921505327	16.2114929487428405	T	T	T
0.0019741142898111	1.0553484711530328	18.9483361562445687	T	T	T
1.4381172289915929	2.4833770579666221	20.9968846666608506	T	T	T
0.0032365338769271	1.0476866722372835	23.0610259029896163	T	T	T
0.0023228196125320	3.9381597567176256	18.9678245060178341	T	T	T
1.4446376556269340	5.3761933223672838	20.9882706149187825	T	T	T
0.0019480436962210	3.9353848454119249	23.0384081125304370	T	T	T
2.9340626302725394	1.0522052450596588	18.9634754379126242	T	T	T
4.3082926993866213	2.5074278548937934	21.0436242077548137	T	T	T
2.8733289481861761	1.0420541882581540	23.0686245155628384	T	T	T
2.8821550030262628	3.9186983653575922	18.9696510342923013	T	T	T
4.3206366121757940	5.3645537825389384	21.0213599280548280	T	T	T
2.8652992475875720	3.9292974270020400	23.0680949156590920	T	T	T
5.7921287457379513	1.1075188831033920	19.0377198836197863	T	T	T
7.2046909660053462	2.5338887745533802	21.0786368318049355	T	T	T
5.7567139884416898	1.0586963314386106	23.0763149306157622	T	T	T
5.7619034798956514	3.9427020336918721	19.0066530165008167	T	T	T
7.2040666670957147	5.3686857950316709	21.0427673128581070	T	T	T
5.7503983706195365	3.9437582701075384	23.1128276442247511	T	T	T
8.6162686797351107	1.1080987498126627	19.0377050105640855	T	T	T
10.1000686059660385	2.5078238363298522	21.0439788260574190	T	T	T
8.6527622771676551	1.0598262597193437	23.0768861773272000	T	T	T
8.6469400250181927	3.9431777554918823	19.0064581745310406	T	T	T
10.0872971976876364	5.3649608648759903	21.0218329309306284	T	T	T

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  8.6573872621916337  3.9450408795468346 23.1131995944604611   T   T   T
 11.4734893159736835  1.0523257847496861 18.9637465175506463   T   T   T
 12.9698374369936964  2.4827576963163791 20.9977110393577604   T   T   T
 11.5351729427962919  1.0416927632681294 23.0689482961709587   T   T   T
 11.5261926607103682  3.9185561047110062 18.9700312388486765   T   T   T
 12.9623842599726160  5.3758220164058592 20.9884247723176571   T   T   T
 11.5413987142502670  3.9292761110396652 23.0688057000131330   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_5x2/Ag E_tot= -277.91246298 eV
 D3-zero damping= -9.7216267 eV, D3-BJ damping= -9.958258 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O
 1.0000000000000000
    14.4026352597500011    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7610541039000012    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.9371186129033156
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.6005703857084863  5.7556662109984709  8.9451241821253618   F   F   F
  1.8002431895326734  2.8751391792884893  8.0000001838787966   F   F   F
  3.6005709759383016  3.5714802856548644  8.9451248436730744   F   F   F
  1.8002421924842598  0.6909532505510081  8.0000000000000000   F   F   F
  1.8002460258749422  5.7556661319886882 11.7805090714841079   F   F   F
  3.6005776446366298  2.8751391002787066 10.8353850732375427   F   F   F
  1.8002466161047572  3.5714802066450821 11.7805097330318205   F   F   F
  3.6005766475882166  0.6909531715412253 10.8353848893587461   F   F   F
  3.6007432355484816  5.6450260727865968 14.3024738882495086   T   T   T
  1.7994665301994839  2.8521329654650196 13.6406583612793497   T   T   T
  3.6007667944705539  3.5734649982718589 14.3154199613066169   T   T   T
  1.7993294479774498  0.6911483160216316 13.6585109813867760   T   T   T
  1.7998549347965191  5.4656325237917409 16.5743757707297306   T   T   T
  3.6008494926487740  2.7893933773606494 16.2729376396601211   T   T   T
  1.7998594859597827  3.5459783027796972 16.7578411754000207   T   T   T
  3.6008335733598629  0.6266146836324799 16.2649688429629222   T   T   T
  7.2012292006459866  5.7556662109984709  8.9451241821253618   F   F   F
  5.4009020044701739  2.8751391792884893  8.0000001838787966   F   F   F
  7.2012297908758027  3.5714802856548644  8.9451248436730744   F   F   F
  5.4009010074217603  0.6909532505510081  8.0000000000000000   F   F   F
  5.4009048408124416  5.7556661319886882 11.7805090714841079   F   F   F
  7.2012364595741305  2.8751391002787066 10.8353850732375427   F   F   F
  5.4009054310422568  3.5714802066450821 11.7805097330318205   F   F   F
  7.2012354625257160  0.6909531715412253 10.8353848893587461   F   F   F
  7.2013973816468955  5.6459199279561458 14.3017963434214934   T   T   T
  5.4021350962722678  2.8520786236208870 13.6406703054888112   T   T   T
  7.2014590823303184  3.5734450396398212 14.3160425491364514   T   T   T
  5.4021769246403206  0.6911418320333778 13.6584994974229126   T   T   T
  5.4018547654878288  5.4654273434941905 16.5743382431518747   T   T   T
  7.2014547784274781  2.7882577060717879 16.2717296036347001   T   T   T
  5.4018199286511965  3.5461399689029962 16.7578332391495231   T   T   T
  7.2015680843007592  0.6269402276199839 16.2660530384198978   T   T   T
 10.8018880155834864  5.7556662109984709  8.9451241821253618   F   F   F
  9.0015608194076737  2.8751391792884893  8.0000001838787966   F   F   F
 10.8018886058133017  3.5714802856548644  8.9451248436730744   F   F   F
  9.0015598223592601  0.6909532505510081  8.0000000000000000   F   F   F
  9.0015636557499441  5.7556661319886882 11.7805090714841079   F   F   F
 10.8018952745116312  2.8751391002787066 10.8353850732375427   F   F   F
  9.0015642459797576  3.5714802066450821 11.7805097330318205   F   F   F
 10.8018942774632194  0.6909531715412253 10.8353848893587461   F   F   F
 10.8020614384507336  5.6450263284642235 14.3024734659890953   T   T   T
  9.0007840907472971  2.8521331807436212 13.6406583206507168   T   T   T
 10.8020847646339728  3.5734653603788447 14.3154191658606109   T   T   T
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  9.0006472523307082  0.6911482194738351 13.6585111951283675   T   T   T
  9.0011739514788758  5.4656330638132395 16.5743738814845649   T   T   T
 10.8021675709158096  2.7893929775058885 16.2729366581940518   T   T   T
  9.0011772811069211  3.5459787426007447 16.7578395479425808   T   T   T
 10.8021551729448237  0.6266210944560766 16.2649713536341416   T   T   T
 14.4025468305209881  5.7556662109984709  8.9451241821253618   F   F   F
 12.6022196343451753  2.8751391792884893  8.0000001838787966   F   F   F
 14.4025474207508051  3.5714802856548644  8.9451248436730744   F   F   F
 12.6022186372967617  0.6909532505510081  8.0000000000000000   F   F   F
 12.6022224706874457  5.7556661319886882 11.7805090714841079   F   F   F
 14.4025540894491328  2.8751391002787066 10.8353850732375427   F   F   F
 12.6022230609172592  3.5714802066450821 11.7805097330318205   F   F   F
 14.4025530924007192  0.6909531715412253 10.8353848893587461   F   F   F
 14.4027156259138938  5.6459200604673221 14.3017973186564991   T   T   T
 12.6034539083464718  2.8520786183415412 13.6406702912825324   T   T   T
 14.4027772144002579  3.5734450943975493 14.3160431339871188   T   T   T
 12.6034949765485180  0.6911418324935527 13.6584994085525793   T   T   T
 12.6031722531588262  5.4654273579201096 16.5743381226456705   T   T   T
 14.4027724843469862  2.7882577548985670 16.2717306129684935   T   T   T
 12.6031376114884885  3.5461403302455761 16.7578329521424010   T   T   T
 14.4028858602496097  0.6269401957064392 16.2660537746163136   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_5x2/Ag E_tot= -81.83418486 eV
 D3-zero damping= -9.0057373 eV, D3-BJ damping= -11.3423328 eV
Ag
 1.0000000000000000
    14.4026352597500011    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7610541039000012    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.8120708806377266
  30
Cartesian
  0.0000041994167452 -0.0000001301627931  7.8535838765487913
  1.4402706569712396  1.4402625283098529  9.9060764030019755
  0.0000025793164628 -0.0000003494199084 11.9584905959405194
  0.0000040130506749  2.8805271239592662  7.8535832156202261
  1.4402723003785656  4.3207915508741150  9.9060765351149076
  0.0000020817251801  2.8805271688868164 11.9584890736084901
  2.8805228336113773 -0.0000003227572619  7.8535659849295856
  4.3207836790513277  1.4402634092964774  9.9060336758254497
  2.8805324994655255 -0.0000003639133359 11.9584856209043320
  2.8805230137002837  2.8805273405656746  7.8535665363343474
  4.3207798368329815  4.3207907158626728  9.9060338757896726
  2.8805328366772014  2.8805274098015290 11.9584856486552038
  5.7610467492383703  0.0000007042940786  7.8535445104129487
  7.2013144399925384  1.4402638369823062  9.9059976164172898
  5.7610546584042277  0.0000010072763071 11.9584538527285975
  5.7610466359673254  2.8805263135143346  7.8535441663669525
  7.2013116606688499  4.3207903336093176  9.9059972870416431
  5.7610536620535582  2.8805260575561191 11.9584539228214872
  8.6415816960202729  0.0000018009937191  7.8535350196704554
 10.0818438507283865  1.4402625366659894  9.9060129019961654
  8.6415802142986919  0.0000023924034282 11.9584396498365653
  8.6415813662082215  2.8805253226168404  7.8535343373200410
 10.0818458728299074  4.3207916443317664  9.9060128614536911
  8.6415812197582493  2.8805250340349522 11.9584394783340890
 11.5221151602631942  0.0000013380858958  7.8535567540164601
 12.9623753093581886  1.4402614349922245  9.9060658382620730
 11.5221007713406411  0.0000013918374884 11.9584628213864050
 11.5221148830850435  2.8805257480056849  7.8535585784798840
 12.9623786245393688  4.3207924491294829  9.9060655870599241
 11.5221010750207213  2.8805256569207196 11.9584618908981959

Interface: ZnO(10-10)/fcc(100)_5x2/Cu E_tot= -402.20160436 eV
```

```
 D3-zero damping= -23.1558071 eV, D3-BJ damping= -26.7376466 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Cu
 1.0000000000000000
    12.6188481836500017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.0475392734600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.1824709295180504
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2  30
Selective dynamics
Cartesian
  3.1546345687705886  5.0428186788376976  8.9451241821253618   F   F   F
  1.5772804832354672  2.5190490598409605  8.0000001838787966   F   F   F
  3.1546350858995926  3.1291473194163189  8.9451248436730744   F   F   F
  1.5772796096729325  0.6053776974460434  8.0000000000000000   F   F   F
  1.5772829682926697  5.0428186096133896 11.7805090714841079   F   F   F
  3.1546409286700490  2.5190489906166529 10.8353850732375427   F   F   F
  1.5772834854216737  3.1291472501920117 11.7805097330318205   F   F   F
  3.1546400551075147  0.6053776282217357 10.8353848893587461   F   F   F
  3.1404693516508919  5.1089858333753257 14.7454984307340613   T   T   T
  1.5707352913367101  2.5763218774842112 13.7062235277464008   T   T   T
  3.1479820394819762  3.1231461711456512 14.7722180731506345   T   T   T
  1.5755438670365705  0.6004058625080857 13.6823129030340169   T   T   T
  1.5179766762314741  5.1787060652629391 17.7724150978828597   T   T   T
  3.1274557168788855  2.6010238015825422 16.6867786033740551   T   T   T
  1.5781266151044935  3.1756933312373588 17.7819138880243379   T   T   T
  3.1009209466063576  0.6174275858370899 16.6461413582405626   T   T   T
  6.3093466146830881  5.0428186788376976  8.9451241821253618   F   F   F
  4.7319925291479681  2.5190490598409605  8.0000001838787966   F   F   F
  6.3093471318120935  3.1291473194163189  8.9451248436730744   F   F   F
  4.7319916555854329  0.6053776974460434  8.0000000000000000   F   F   F
  4.7319950142051699  5.0428186096133896 11.7805090714841079   F   F   F
  6.3093529745825494  2.5190489906166529 10.8353850732375427   F   F   F
  4.7319955313341735  3.1291472501920117 11.7805097330318205   F   F   F
  6.3093521010200142  0.6053776282217357 10.8353848893587461   F   F   F
  6.3093951524420149  5.1041902438384446 14.7326492497477428   T   T   T
  4.7206593439590305  2.5702492434792670 13.7021835052830756   T   T   T
  6.3093993169602962  3.1192993300338832 14.7421537528838513   T   T   T
  4.7232181000560836  0.5918012040426611 13.6946023355186295   T   T   T
  4.6924265684400330  5.1199697516709906 17.6584417228816903   T   T   T
  6.3097394813850949  2.5870085323882672 16.6490010745572370   T   T   T
  4.7401312200009560  3.1355156087554290 17.6903843494326658   T   T   T
  6.3095136175735940  0.6016608315276678 16.6399608631942186   T   T   T
  9.4640586605955885  5.0428186788376976  8.9451241821253618   F   F   F
  7.8867045750604676  2.5190490598409605  8.0000001838787966   F   F   F
  9.4640591777245930  3.1291473194163189  8.9451248436730744   F   F   F
  7.8867037014979324  0.6053776974460434  8.0000000000000000   F   F   F
  7.8867070601176712  5.0428186096133896 11.7805090714841079   F   F   F
  9.4640650204950507  2.5190489906166529 10.8353850732375427   F   F   F
  7.8867075772466739  3.1291472501920117 11.7805097330318205   F   F   F
  9.4640641469325164  0.6053776282217357 10.8353848893587461   F   F   F
  9.4783877617309642  5.1091305738388604 14.7455431230323146   T   T   T
  7.8982511822444010  2.5703457076239506 13.7022447469514255   T   T   T
  9.4708401253932504  3.1233264843906703 14.7722828146026011   T   T   T
  7.8956052156758929  0.5918769692296673 13.6946601517019211   T   T   T
  7.9266376368241991  5.1200586784225823 17.6582535136886527   T   T   T
  9.4921347574030204  2.6011250792053171 16.6868715656984961   T   T   T
  7.8793100064019583  3.1356890271811566 17.6901949776994023   T   T   T
  9.5183683100758500  0.6175011012362450 16.6461894227009921   T   T   T
 12.6187707065080907  5.0428186788376976  8.9451241821253618   F   F   F
 11.0414166209729689  2.5190490598409605  8.0000001838787966   F   F   F
 12.6187712236370952  3.1291473194163189  8.9451248436730744   F   F   F
 11.0414157474104346  0.6053776974460434  8.0000000000000000   F   F   F
```

```
 11.0414191060301725  5.0428186096133896 11.7805090714841079   F   F   F
 12.6187770664075511  2.5190489906166529 10.8353850732375427   F   F   F
 11.0414196231591752  3.1291472501920117 11.7805097330318205   F   F   F
 12.6187761928450186  0.6053776282217357 10.8353848893587461   F   F   F
 12.6188766686448055  5.1117486411025457 14.7309366506663455   T   T   T
 11.0480252889573904  2.5764232521421029 13.7062093902889295   T   T   T
 12.6188540960112583  3.1280587947638949 14.7832452466804423   T   T   T
 11.0433799791563771  0.6004803479744818 13.6823095308929901   T   T   T
 11.1015668879201499  5.1789951410528046 17.7721556353419423   T   T   T
 12.6192546994166239  2.6165335590763168 16.7009452697062422   T   T   T
 11.0414234376983238  3.1758826462596619 17.7816279371906809   T   T   T
 12.6192514139744549  0.6387375067745832 16.6129524859349331   T   T   T
  0.0006808906013226  0.8058071455273259 19.7888137191962734   T   T   T
  1.2489922039801098  2.1164411181721721 21.5496330446894362   T   T   T
  0.0007113237615596  0.8289941850617419 23.3263875806520353   T   T   T
  0.0008049817839911  3.3284453513288983 19.6792606996825405   T   T   T
  1.2585243765385874  4.5999337480272064 21.5470650643353601   T   T   T
  0.0007115396800062  3.3573658533743336 23.3443478824607702   T   T   T
  2.5713388028782180  0.8546965858553363 19.8565382310403962   T   T   T
  3.7690289370411807  2.1801652530511677 21.5778098138766730   T   T   T
  2.5165684342562678  0.8560164505833504 23.3220827621503055   T   T   T
  2.4774409710144814  3.3637734548913358 19.6790655382844122   T   T   T
  3.7849839155448595  4.6234712777472895 21.5656833202246325   T   T   T
  2.5102881216439834  3.3835501303981932 23.3592425916934374   T   T   T
  5.0688389564457443  0.9264764794097172 19.9076404010831851   T   T   T
  6.3101531476868047  2.2164355730241230 21.5905532922000383   T   T   T
  5.0446632737355257  0.8966758474385434 23.3191778213662744   T   T   T
  5.0193989422659540  3.4284250579476070 19.6788574661400553   T   T   T
  6.3101346456578202  4.6434173298910162 21.5708208548814042   T   T   T
  5.0411105878627556  3.4219500142565251 23.3813095889466993   T   T   T
  7.5515096789283911  0.9263859598506172 19.9076523166676260   T   T   T
  8.8512551306950318  2.1801275372105731 21.5776977581738265   T   T   T
  7.5756226225249019  0.8966414033349550 23.3191139984631164   T   T   T
  7.6007972104969461  3.4283812244295206 19.6787337789852899   T   T   T
  8.8353293831694089  4.6233547516622666 21.5655698041587378   T   T   T
  7.5792293478973320  3.4219117831860597 23.3812492743230749   T   T   T
 10.0490444613923184  0.8547027680462711 19.8566152591264036   T   T   T
 11.3713471294016468  2.1164844295257934 21.5495584526064761   T   T   T
 10.1036971740177748  0.8559626235376470 23.3219311265964997   T   T   T
 10.1429721327927975  3.3637292684549611 19.6788715286566500   T   T   T
 11.3618213049388359  4.5999101269550655 21.5470386704322330   T   T   T
 10.1099844475861271  3.3835068699815265 23.3591108022040252   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_5x2/Cu E_tot= -285.70205649 eV
 D3-zero damping= -10.8667327 eV, D3-BJ damping= -12.2036999 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O
 1.0000000000000000
    12.6188481836500017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.0475392734600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.9371186129033156
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.1546345687705886  5.0428186788376976  8.9451241821253618   F   F   F
  1.5772804832354672  2.5190490598409605  8.0000001838787966   F   F   F
  3.1546350858995926  3.1291473194163189  8.9451248436730744   F   F   F
  1.5772796096729325  0.6053776974460434  8.0000000000000000   F   F   F
  1.5772829682926697  5.0428186096133896 11.7805090714841079   F   F   F
  3.1546409286700490  2.5190489906166529 10.8353850732375427   F   F   F
  1.5772834854216737  3.1291472501920117 11.7805097330318205   F   F   F
  3.1546400551075147  0.6053776282217357 10.8353848893587461   F   F   F
```

```
  3.1548902862426114  5.0880147856869939 14.6970284474373472   T   T   T
  1.5773542472789748  2.5834818434315374 13.7219480347460365   T   T   T
  3.1550000249084356  3.1113409748648038 14.7872081164450559   T   T   T
  1.5773605493359519  0.6030896422349041 13.6806393773437218   T   T   T
  1.5781076315408169  4.8846245341177106 17.4277455375899279   T   T   T
  3.1548743072403362  2.5723498616804878 16.7648464081819064   T   T   T
  1.5778989970704054  3.0571427675633029 17.7835696662097043   T   T   T
  3.1552730346210303  0.6040134628703939 16.6261465493078155   T   T   T
  6.3093466146830881  5.0428186788376976  8.9451241821253618   F   F   F
  4.7319925291479681  2.5190490598409605  8.0000001838787966   F   F   F
  6.3093471318120935  3.1291473194163189  8.9451248436730744   F   F   F
  4.7319916555854329  0.6053776974460434  8.0000000000000000   F   F   F
  4.7319950142051699  5.0428186096133896 11.7805090714841079   F   F   F
  6.3093529745825494  2.5190489906166529 10.8353850732375427   F   F   F
  4.7319955313341735  3.1291472501920117 11.7805097330318205   F   F   F
  6.3093521010200142  0.6053776282217357 10.8353848893587461   F   F   F
  6.3095034414929829  5.0880189065323425 14.6975690817536346   T   T   T
  4.7327670113346958  2.5836978535124473 13.7219164919544401   T   T   T
  6.3097771231427346  3.1113794417065215 14.7881555246905094   T   T   T
  4.7323825134320225  0.6033278227426119 13.6805958011132844   T   T   T
  4.7325718551242781  4.8847004402664265 17.4276809373977173   T   T   T
  6.3096738416471609  2.5722253906430526 16.7662190734694576   T   T   T
  4.7318819571530124  3.0571558561262360 17.7834293177239253   T   T   T
  6.3100002736499921  0.6039700710878660 16.6266124491071707   T   T   T
  9.4640586605955885  5.0428186788376976  8.9451241821253618   F   F   F
  7.8867045750604676  2.5190490598409605  8.0000001838787966   F   F   F
  9.4640591777245930  3.1291473194163189  8.9451248436730744   F   F   F
  7.8867037014979324  0.6053776974460434  8.0000000000000000   F   F   F
  7.8867070601176712  5.0428186096133896 11.7805090714841079   F   F   F
  9.4640650204950507  2.5190489906166529 10.8353850732375427   F   F   F
  7.8867075772466739  3.1291472501920117 11.7805097330318205   F   F   F
  9.4640641469325164  0.6053776282217357 10.8353848893587461   F   F   F
  9.4642175858326247  5.0881178696672444 14.6969839922469401   T   T   T
  7.8868293234669631  2.5836398835523244 13.7219045347001174   T   T   T
  9.4644474917219803  3.1114650712413505 14.7872528276792945   T   T   T
  7.8867294760289344  0.6032802997703677 13.6805621570724085   T   T   T
  7.8875520520115998  4.8846415378256269 17.4277274812800727   T   T   T
  9.4643226755746870  2.5723415809814849 16.7648963621049738   T   T   T
  7.8873133299121925  3.0571625772159723 17.7835563818817377   T   T   T
  9.4647094612587406  0.6040180572798872 16.6261057183696686   T   T   T
 12.6187707065080907  5.0428186788376976  8.9451241821253618   F   F   F
 11.0414166209729689  2.5190490598409605  8.0000001838787966   F   F   F
 12.6187712236370952  3.1291473194163189  8.9451248436730744   F   F   F
 11.0414157474104346  0.6053776974460434  8.0000000000000000   F   F   F
 11.0414191060301725  5.0428186096133896 11.7805090714841079   F   F   F
 12.6187770664075511  2.5190489906166529 10.8353850732375427   F   F   F
 11.0414196231591752  3.1291472501920117 11.7805097330318205   F   F   F
 12.6187761928450186  0.6053776282217357 10.8353848893587461   F   F   F
 12.6188890449941855  5.0879958830185030 14.6976200219109945   T   T   T
 11.0421661616318190  2.5837139510105276 13.7219330247411726   T   T   T
 12.6191545261316396  3.1113558243910640 14.7882208353234699   T   T   T
 11.0418103874208171  0.6033432900104038 13.6805845515817932   T   T   T
 11.0419563031063781  4.8847157402579837 17.4277688333245457   T   T   T
 12.6190636107992979  2.5722178398617661 16.7662934003608726   T   T   T
 11.0412940960608577  3.0571691332031850 17.7835243500963358   T   T   T
 12.6193889804404407  0.6039591253269492 16.6266659158985313   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_5x2/Cu E_tot= -108.83879644 eV
 D3-zero damping= -8.5936592 eV, D3-BJ damping= -10.8758952 eV
Cu
 1.0000000000000000
    12.6188481836500017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.0475392734600009    0.0000000000000000
```

```
     0.0000000000000000    0.0000000000000000   19.8120708806377266
  30
Cartesian
  0.0000035952627925  0.0000005782701361  8.1194781907459355
  1.2623972624690907  1.2618842233915910  9.9060633349368565
  0.0000027041124978  0.0000005235010132 11.6925870034654800
  0.0000032244892430  2.5237690338578065  8.1194777997224286
  1.2623960512684840  3.7856550559217426  9.9060633967878982
  0.0000017045357664  2.5237689274310302 11.6925865665212392
  2.5238395289147322 -0.0000016885529254  8.1197048341660949
  3.7851238659684912  1.2618846409816624  9.9060301144938006
  2.5238424735434508 -0.0000016525974995 11.6923440924423883
  2.5238396126088527  2.5237712953698250  8.1197048411011181
  3.7851236635336307  3.7856546511045166  9.9060301457649800
  2.5238439629281886  2.5237712840164543 11.6923438788094689
  5.0471149807546629  0.0000019108028326  8.1194314830117271
  6.3094234441187060  1.2618848708288810  9.9060033103578817
  5.0471192275194747  0.0000020148646494 11.6925781241830098
  5.0471149342875199  2.5237676960140698  8.1194313310091069
  6.3094218772990258  3.7856544038256956  9.9060029174334083
  5.0471179000758379  2.5237676331522709 11.6925779571048682
  7.5717292435847234  0.0000033754109706  8.1194236641290445
  8.8337192501256521  1.2618843885329589  9.9060131738417176
  7.5717276949941619  0.0000035218177569 11.6925687871793791
  7.5717291760696641  2.5237661421352029  8.1194234339976958
  8.8337196451242459  3.7856549261270560  9.9060130821542760
  7.5717286809542852  2.5237661980350548 11.6925688751915526
 10.0950095343551585  0.0000016681553244  8.1196955127134185
 11.3564564272653570  1.2618836528446338  9.9060548698355326
 10.0950035379177319  0.0000019733380796 11.6923287880638895
 10.0950098961299943  2.5237679984877719  8.1196961700029799
 11.3564591188363462  3.7856555811413171  9.9060546612956237
 10.0950039705149592  2.5237676605954342 11.6923281473677161

Interface: ZnO(10-10)/fcc(100)_5x2/Pt E_tot= -473.85406302 eV
 D3-zero damping= -29.3155467 eV, D3-BJ damping= -29.0106021 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Pt
 1.0000000000000000
    13.8522668271000011    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.5409067308400006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.1824709295180504
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2  30
Selective dynamics
Cartesian
  3.4629816566953777  5.5357247256887341  8.9451241821253618   F   F   F
  1.7314504301005962  2.7652713797353203  8.0000001838787966   F   F   F
  3.4629822243707191  3.4350031777085537  8.9451248436730744   F   F   F
  1.7314494711524302  0.6645498284909550  8.0000000000000000   F   F   F
  1.7314531580576131  5.5357246496981549 11.7805090714841079   F   F   F
  3.4629886382378321  2.7652713037447412 10.8353850732375427   F   F   F
  1.7314537257329545  3.4350031017179750 11.7805097330318205   F   F   F
  3.4629876792896663  0.6645497525003760 10.8353848893587461   F   F   F
  3.4362016463481533  5.4647142207412767 14.4157406807037987   T   T   T
  1.6983004151214502  2.7414116938770134 13.6733237475180349   T   T   T
  3.4624317179837583  3.4366165781856162 14.4514086518324660   T   T   T
  1.7153345441425538  0.6832375176024152 13.6543831137945464   T   T   T
  1.6836931133991511  5.6482918003153451 17.1809753178563120   T   T   T
  3.5065219578582383  2.7132618014273282 16.3436326143452284   T   T   T
  1.8522328798991190  3.5925201945051946 17.1004466151298118   T   T   T
  3.4443046688086740  0.7140155330415786 16.2681508682766420   T   T   T
  6.9260483634703771  5.5357247256887341  8.9451241821253618   F   F   F
```

5.1945171368755965	2.7652713797353203	8.0000001838787966	F	F	F
6.9260489311457203	3.4350031777085537	8.9451248436730744	F	F	F
5.1945161779274311	0.6645498284909550	8.0000000000000000	F	F	F
5.1945198648326123	5.5357246496981549	11.7805090714841079	F	F	F
6.9260553450128324	2.7652713037447412	10.8353850732375427	F	F	F
5.1945204325079546	3.4350031017179750	11.7805097330318205	F	F	F
6.9260543860646662	0.6645497525003760	10.8353848893587461	F	F	F
6.9261062109619616	5.4430849284139411	14.3801406638604394	T	T	T
5.1811192898229033	2.7086885625794217	13.6279123815882723	T	T	T
6.9261001302074083	3.4219562028920976	14.4104910287898971	T	T	T
5.1827808626456351	0.6629923694773294	13.6578173890483594	T	T	T
5.1713464501063617	5.5839364683897585	17.0159398049665320	T	T	T
6.9259588181981551	2.6794900157459929	16.2870331860428479	T	T	T
5.2513807117411595	3.5389711806853690	17.0031004528510969	T	T	T
6.9260915171308053	0.6889475933876011	16.2342830745004072	T	T	T
10.3891150702453778	5.5357247256887341	8.9451241821253618	F	F	F
8.6575838436505954	2.7652713797353203	8.0000001838787966	F	F	F
10.3891156379207192	3.4350031777085537	8.9451248436730744	F	F	F
8.6575828847024301	0.6645498284909550	8.0000000000000000	F	F	F
8.6575865716076148	5.5357246496981549	11.7805090714841079	F	F	F
10.3891220517878331	2.7652713037447412	10.8353850732375427	F	F	F
8.6575871392829544	3.4350031017179750	11.7805097330318205	F	F	F
10.3891210928396678	0.6645497525003760	10.8353848893587461	F	F	F
10.4158924694446551	5.4646575964417199	14.4155952867329944	T	T	T
8.6709690734235867	2.7086398856168352	13.6278319292274706	T	T	T
10.3894962507508808	3.4366410482818508	14.4514457944947754	T	T	T
8.6693161132607095	0.6630134951422096	13.6577919477756335	T	T	T
8.6807212932199214	5.5839549526557679	17.0160792236751135	T	T	T
10.3450528748913584	2.7130606781309883	16.3434963411525160	T	T	T
8.6005357362582888	3.5391139433265475	17.0029252246126745	T	T	T
10.4075499856725777	0.7139802537197303	16.2680299027904240	T	T	T
13.8521817770203786	5.5357247256887341	8.9451241821253618	F	F	F
12.1206505504255979	2.7652713797353203	8.0000001838787966	F	F	F
13.8521823446957217	3.4350031777085537	8.9451248436730744	F	F	F
12.1206495914774308	0.6645498284909550	8.0000000000000000	F	F	F
12.1206532783826155	5.5357246496981549	11.7805090714841079	F	F	F
13.8521887585628338	2.7652713037447412	10.8353850732375427	F	F	F
12.1206538460579551	3.4350031017179750	11.7805097330318205	F	F	F
13.8521877996146703	0.6645497525003760	10.8353848893587461	F	F	F
13.8520565247911360	5.4916059740046324	14.4553325689047973	T	T	T
12.1534197812003022	2.7414572601337377	13.6732509825282094	T	T	T
13.8519953545865935	3.4556038631851727	14.5883050811458226	T	T	T
12.1366594879334055	0.6832587263537879	13.6543617734545304	T	T	T
12.1679382980824791	5.6483132291165195	17.1811012174980924	T	T	T
13.8518570908975018	2.8111620304421727	16.5789360510219801	T	T	T
11.9992685029994473	3.5925715864558931	17.1003578522995205	T	T	T
13.8519393583655095	0.7838697220219633	16.2894189982408868	T	T	T
-0.0002246716555676	0.6607159556596330	19.3240146275681361	T	T	T
1.3792009316624567	2.0752703195695146	21.3411625701425578	T	T	T
-0.0005257246519414	0.7054236555365854	23.3620383341425715	T	T	T
-0.0003470149319469	3.4312080181392428	19.4712481114898175	T	T	T
1.3841394548307726	4.8538080093743252	21.3339784768046918	T	T	T
-0.0005408776379401	3.4802274373062430	23.2581244006279100	T	T	T
2.7667841135040603	0.6681026688552839	19.4028176016172473	T	T	T
4.1155826603345629	2.1907215493346466	21.1928608821130062	T	T	T
2.7926767799892454	0.7382441030961925	23.2078222625328543	T	T	T
2.6747163455736804	3.3664885332018484	19.0716027355743236	T	T	T
4.1443052743813134	4.8553949396597709	21.2476696752831167	T	T	T
2.8006338373873527	3.5009955540203110	23.2638472089189321	T	T	T
5.5419606080362085	0.7088298694160715	19.3878666004115097	T	T	T
6.9257923917548787	2.2072490464146983	21.1897238210796566	T	T	T
5.5375250212733205	0.8027615069853634	23.1455523377619343	T	T	T
5.4903402810335047	3.4135149270548397	19.0804848264562246	T	T	T

```
  6.9255276940353507  4.8745787764932773 21.2395911794536474   T   T   T
  5.5396758437213638  3.5366726529943247 23.1858673840795220   T   T   T
  8.3093965649728361  0.7085564252466037 19.3880084741578607   T   T   T
  9.7355110776631140  2.1908493180397968 21.1931295599416671   T   T   T
  8.3131094747595373  0.8026329400497305 23.1458076733555806   T   T   T
  8.3617078502859865  3.4135440784602342 19.0805225643656335   T   T   T
  9.7068872909245005  4.8554674053741316 21.2479754609139420   T   T   T
  8.3113629434362917  3.5366300703872016 23.1857413832689900   T   T   T
 11.0844217394593620  0.6682004057482834 19.4030866553975798   T   T   T
 12.4725228688018213  2.0752286710116206 21.3410625967980323   T   T   T
 11.0583823017936975  0.7385648906124727 23.2078036475684506   T   T   T
 11.1769251736774091  3.3663510411944357 19.0716227444891473   T   T   T
 12.4673326641327051  4.8539658615957730 21.3338901849971592   T   T   T
 11.0509400707606815  3.5012123385376306 23.2638646440952925   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_5x2/Pt E_tot= -284.46714892 eV
 D3-zero damping= -10.0516655 eV, D3-BJ damping= -10.5913449 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O
 1.0000000000000000
    13.8522668271000011    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.5409067308400006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.9371186129033156
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.4629816566953777  5.5357247256887341  8.9451241821253618   F   F   F
  1.7314504301005962  2.7652713797353203  8.0000001838787966   F   F   F
  3.4629822243707191  3.4350031777085537  8.9451248436730744   F   F   F
  1.7314494711524302  0.6645498284909550  8.0000000000000000   F   F   F
  1.7314531580576131  5.5357246496981549 11.7805090714841079   F   F   F
  3.4629886382378321  2.7652713037447412 10.8353850732375427   F   F   F
  1.7314537257329545  3.4350031017179750 11.7805097330318205   F   F   F
  3.4629876792896663  0.6645497525003760 10.8353848893587461   F   F   F
  3.4630652282929564  5.4400367440923034 14.3971121426914248   T   T   T
  1.7315826595193746  2.7337869087141606 13.6630201527592199   T   T   T
  3.4630713412234893  3.4184725809474368 14.4396901975445342   T   T   T
  1.7308193655070319  0.6616823304441972 13.6728811880414245   T   T   T
  1.7317942994158488  5.2680447461390241 16.7774895036963230   T   T   T
  3.4631117792316335  2.6838353330966123 16.4262565414729913   T   T   T
  1.7306693661375776  3.3882857808487392 17.0278922550249447   T   T   T
  3.4632044605281580  0.6147363470346222 16.3692211874419442   T   T   T
  6.9260483634703771  5.5357247256887341  8.9451241821253618   F   F   F
  5.1945171368755965  2.7652713797353203  8.0000001838787966   F   F   F
  6.9260489311457203  3.4350031777085537  8.9451248436730744   F   F   F
  5.1945161779274311  0.6645498284909550  8.0000000000000000   F   F   F
  5.1945198648326123  5.5357246496981549 11.7805090714841079   F   F   F
  6.9260553450128324  2.7652713037447412 10.8353850732375427   F   F   F
  5.1945204325079546  3.4350031017179750 11.7805097330318205   F   F   F
  6.9260543860646662  0.6645497525003760 10.8353848893587461   F   F   F
  6.9261101139888082  5.4386882571874144 14.3960955891965714   T   T   T
  5.1945536157722421  2.7337561401564754 13.6630206449418115   T   T   T
  6.9261364969142063  3.4178626904066558 14.4401767060960395   T   T   T
  5.1952942164367819  0.6616734082438094 13.6728606680251641   T   T   T
  5.1945435523859969  5.2679718492102952 16.7776157950269891   T   T   T
  6.9262704708063270  2.6801283920742613 16.4254980226314018   T   T   T
  5.1956872629819237  3.3881945116979990 17.0278424622529876   T   T   T
  6.9262085833332767  0.6136058059475537 16.3686621007766391   T   T   T
 10.3891150702453778  5.5357247256887341  8.9451241821253618   F   F   F
  8.6575838436505954  2.7652713797353203  8.0000001838787966   F   F   F
 10.3891156379207192  3.4350031777085537  8.9451248436730744   F   F   F
  8.6575828847024301  0.6645498284909550  8.0000000000000000   F   F   F
```

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  8.6575865716076148  5.5357246496981549 11.7805090714841079   F   F   F
 10.3891220517878331  2.7652713037447412 10.8353850732375427   F   F   F
  8.6575871392829544  3.4350031017179750 11.7805097330318205   F   F   F
 10.3891210928396678  0.6645497525003760 10.8353848893587461   F   F   F
 10.3891990603843265  5.4400366434677965 14.3971112673790049   T   T   T
  8.6577160521057177  2.7337868870168616 13.6630201035362280   T   T   T
 10.3892050804005898  3.4184725092267310 14.4396896185340591   T   T   T
  8.6569527268144189  0.6616822638500247 13.6728811320056227   T   T   T
  8.6579277557051295  5.2680449054679936 16.7774873629215477   T   T   T
 10.3892454780229126  2.6838353075067145 16.4262556554992969   T   T   T
  8.6568029543485014  3.3882859508089878 17.0278909369259601   T   T   T
 10.3893381443154187  0.6147364502235574 16.3692200799145660   T   T   T
 13.8521817770203786  5.5357247256887341  8.9451241821253618   F   F   F
 12.1206505504255979  2.7652713797353203  8.0000001838787966   F   F   F
 13.8521823446957217  3.4350031777085537  8.9451248436730744   F   F   F
 12.1206495914774308  0.6645498284909550  8.0000000000000000   F   F   F
 12.1206532783826155  5.5357246496981549 11.7805090714841079   F   F   F
 13.8521887585628338  2.7652713037447412 10.8353850732375427   F   F   F
 12.1206538460579551  3.4350031017179750 11.7805097330318205   F   F   F
 13.8521877996146703  0.6645497525003760 10.8353848893587461   F   F   F
 13.8522442013069149  5.4386881774318159 14.3960962995427000   T   T   T
 12.1206875617888858  2.7337558757847971 13.6630205539363399   T   T   T
 13.8522701214424355  3.4178626057478034 14.4401771239210674   T   T   T
 12.1214283206740348  0.6616732748156707 13.6728606870085301   T   T   T
 12.1206768893771653  5.2679717153315329 16.7776152926667237   T   T   T
 13.8524040087988034  2.6801281999017994 16.4254985290057469   T   T   T
 12.1218207146420145  3.3881944788796381 17.0278423124299145   T   T   T
 13.8523422166759946  0.6136056898281512 16.3686627717047344   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_5x2/Pt E_tot= -179.21065265 eV
 D3-zero damping= -13.7487299 eV, D3-BJ damping= -14.4084745 eV
Pt
 1.0000000000000000
    13.8522668271000011    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.5409067308400006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.8120708806377266
  30
Cartesian
  0.0000002048000128 -0.0000006031814036  7.9595550353009443
  1.3852349467085767  1.3852256685380604  9.9060806579199845
  0.0000027062153751 -0.0000007679071881 11.8525481343251986
  0.0000013971665868  2.7704538193953026  7.9595505625816312
  1.3852362335496018  4.1556809465280669  9.9060804456692768
  0.0000037552848192  2.7704539158588148 11.8525457436147601
  2.7704534213195311  0.0000004964838930  7.9595234704701614
  4.1556721919455573  1.3852268237688399  9.9060312079038670
  2.7704546396749508  0.0000001158248468 11.8525362986566893
  2.7704530800933997  2.7704528503849697  7.9595242184228150
  4.1556689432992568  4.1556799126061472  9.9060313083315066
  2.7704535562244086  2.7704532437649894 11.8525359538072070
  5.5409051358591670 -0.0000002304465114  7.9594986602689941
  6.9261291740379622  1.3852269850178462  9.9059887867540901
  5.5409034414339269  0.0000001942828004 11.8524973441543668
  5.5409061199558396  2.7704535630295815  7.9594989334558868
  6.9261270394153849  4.1556797906405514  9.9059889494395303
  5.5409039473798671  2.7704531835273460 11.8524957953008006
  8.3113594485498687  0.0000003412166666  7.9594851684633392
  9.6965857624977598  1.3852258372478403  9.9060041534214722
  8.3113595808501159  0.0000012032660912 11.8524735450232033
  8.3113579795640966  2.7704528789697802  7.9594803781436410
  9.6965874203336249  4.1556810610185702  9.9060041442300175
  8.3113594204731296  2.7704525217860039 11.8524755494467975
 11.0818152888882953  0.0000007181244162  7.9595103746434335
```

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 12.4670449587933074  1.3852248821717073  9.9060676784976955
 11.0818135534434496  0.0000008679427785 11.8525085500083520
 11.0818143123719786  2.7704526801325140  7.9595165673771122
 12.4670475407876875  4.1556818053358864  9.9060673619922621
 11.0818134258603056  2.7704524944073956 11.8525030445760802

Interface: ZnO(10-10)/fcc(100)_5x2/Pd E_tot= -447.17766716 eV
 D3-zero damping= -25.5070375 eV, D3-BJ damping= -27.0700527 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Pd
 1.0000000000000000
    13.7399061595000003    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4959624638000006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.1824709295180504
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2  30
Selective dynamics
Cartesian
  3.4348921796668508  5.4908224917372941  8.9451241821253618   F   F   F
  1.7174060192708966  2.7428412791459800  8.0000001838787966   F   F   F
  3.4348927427375755  3.4071406440833432  8.9451248436730744   F   F   F
  1.7174050681011006  0.6591594282543216  8.0000000000000000   F   F   F
  1.7174087251004830  5.4908224163631019 11.7805090714841079   F   F   F
  3.4348991045795292  2.7428412037717878 10.8353850732375427   F   F   F
  1.7174092881712075  3.4071405687091514 11.7805097330318205   F   F   F
  3.4348981534097334  0.6591593528801291 10.8353848893587461   F   F   F
  3.4171629027964103  5.4394441721767253 14.4398922330741559   T   T   T
  1.7063114095358760  2.7281952692225855 13.6689614510632289   T   T   T
  3.4329288587196354  3.4205923094787711 14.4854954900105906   T   T   T
  1.7064727150268353  0.6809220247443299 13.6605920415925333   T   T   T
  1.6835687982388980  5.5772167555478172 17.1777298031012791   T   T   T
  3.4477283661121536  2.7403558111478157 16.4103900953877826   T   T   T
  1.7623536144660674  3.5746895626349677 17.1136368528161391   T   T   T
  3.4161104189964897  0.7356231985642313 16.3072886313475998   T   T   T
  6.8698687195418504  5.4908224917372941  8.9451241821253618   F   F   F
  5.1523825591458969  2.7428412791459800  8.0000001838787966   F   F   F
  6.8698692826125765  3.4071406440833432  8.9451248436730744   F   F   F
  5.1523816079761007  0.6591594282543216  8.0000000000000000   F   F   F
  5.1523852649754822  5.4908224163631019 11.7805090714841079   F   F   F
  6.8698756444545293  2.7428412037717878 10.8353850732375427   F   F   F
  5.1523858280462074  3.4071405687091514 11.7805097330318205   F   F   F
  6.8698746932847330  0.6591593528801291 10.8353848893587461   F   F   F
  6.8700356602953407  5.4237883999314196 14.4217777021472315   T   T   T
  5.1452924021565769  2.7120088975606262 13.6510530825929841   T   T   T
  6.8700024263593908  3.4089598751010364 14.4564971070709269   T   T   T
  5.1445758753926185  0.6676204009359132 13.6649472781085013   T   T   T
  5.1253971958013107  5.5350831090812234 17.0498916380630305   T   T   T
  6.8701282961755084  2.7017700977445038 16.3697596945683479   T   T   T
  5.1823595507854066  3.5314871501977376 17.0308337181522305   T   T   T
  6.8699925653183174  0.7065289659423436 16.2933784906779273   T   T   T
 10.3048452594168509  5.4908224917372941  8.9451241821253618   F   F   F
  8.5873590990208957  2.7428412791459800  8.0000001838787966   F   F   F
 10.3048458224875752  3.4071406440833432  8.9451248436730744   F   F   F
  8.5873581478511003  0.6591594282543216  8.0000000000000000   F   F   F
  8.5873618048504845  5.4908224163631019 11.7805090714841079   F   F   F
 10.3048521843295298  2.7428412037717878 10.8353850732375427   F   F   F
  8.5873623679212070  3.4071405687091514 11.7805097330318205   F   F   F
 10.3048512331597344  0.6591593528801291 10.8353848893587461   F   F   F
 10.3228885659155090  5.4394221306341866 14.4399286191340579   T   T   T
  8.5946691086779978  2.7119988333075256 13.6511425249005640   T   T   T
 10.3070338154147567  3.4205799898259661 14.4854951924760691   T   T   T
  8.5954987870673918  0.6675856115755380 13.6649817432443808   T   T   T
  8.6147445063031061  5.5351488472477639 17.0498187902345855   T   T   T
```

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 10.2924848572257268  2.7402919362566047 16.4103984905659601   T   T   T
  8.5577976977228118  3.5315326816926675 17.0307750663649173   T   T   T
 10.3240086227782282  0.7355715448723649 16.3072775572627293   T   T   T
 13.7398217992918514  5.4908224917372941  8.9451241821253618   F   F   F
 12.0223356388958980  2.7428412791459800  8.0000001838787966   F   F   F
 13.7398223623625775  3.4071406440833432  8.9451248436730744   F   F   F
 12.0223346877261008  0.6591594282543216  8.0000000000000000   F   F   F
 12.0223383447254850  5.4908224163631019 11.7805090714841079   F   F   F
 13.7398287242045303  2.7428412037717878 10.8353850732375427   F   F   F
 12.0223389077962075  3.4071405687091514 11.7805097330318205   F   F   F
 13.7398277730347367  0.6591593528801291 10.8353848893587461   F   F   F
 13.7399494850540567  5.4520439066184876 14.4594832140584284   T   T   T
 12.0336799036807491  2.7282025478048917 13.6689972185752193   T   T   T
 13.7399339401591778  3.4311148846445523 14.5385510314256976   T   T   T
 12.0335494385492137  0.6809375250562190 13.6605637201215675   T   T   T
 12.0565266195447673  5.5771038350098143 17.1776348383057567   T   T   T
 13.7401105757958284  2.7958511316159012 16.4917949287254118   T   T   T
 11.9778071807604345  3.5745862441402272 17.1136506784223528   T   T   T
 13.7400493307054603  0.7731048482253086 16.3193090901898934   T   T   T
  0.0001531822443247  0.9979210660456155 19.2000401530945020   T   T   T
  1.3743233071759973  2.3667727838746782 21.1966006852728128   T   T   T
  0.0001327761882916  0.9926007824446654 23.1856616114988761   T   T   T
  0.0000429396919063  3.7427045224672661 19.2831268035686278   T   T   T
  1.3777758901981407  5.1258380921117750 21.1893630209710082   T   T   T
  0.0001298327821176  3.7434435479124932 23.1279425863103505   T   T   T
  2.7800054526766234  1.0333202961525487 19.2731692307749718   T   T   T
  4.1133691309835836  2.4223471974355104 21.2044654280866993   T   T   T
  2.7389682416832897  1.0022662709078902 23.1400592252416928   T   T   T
  2.7332909163780372  3.7466559969445874 19.1316919463687256   T   T   T
  4.1175276070273821  5.1114716102509856 21.1693137423329709   T   T   T
  2.7459291564836472  3.7589518442432817 23.1646538863832419   T   T   T
  5.5143782380895585  1.0716845864820086 19.3065052943943876   T   T   T
  6.8701232645581261  2.4392897721453588 21.2222687701387152   T   T   T
  5.4868602702864822  1.0129676958011373 23.1230982817644843   T   T   T
  5.4921596052261998  3.7741487018636652 19.1239336137417766   T   T   T
  6.8700799136285324  5.1126740654106628 21.1692980668645738   T   T   T
  5.4930962279927575  3.7812357574431235 23.1761186843514899   T   T   T
  8.2256828255065209  1.0716882442755749 19.3065202954186041   T   T   T
  9.6267274241764884  2.4222417928451030 21.2045213749940444   T   T   T
  8.2531926740323396  1.0129473158828513 23.1231395863089517   T   T   T
  8.2481112465984552  3.7742621726088181 19.1239157044576871   T   T   T
  9.6227077574432087  5.1114274304260974 21.1693718860051234   T   T   T
  8.2471249756560727  3.7811604996754213 23.1761343361906000   T   T   T
 10.9600803585812638  1.0331877944275547 19.2730528086947892   T   T   T
 12.3658054229249057  2.3666499480562395 21.1965702061940675   T   T   T
 11.0012343103135564  1.0021292755337017 23.1400625922378360   T   T   T
 11.0066075561580980  3.7465496331680948 19.1317024441405188   T   T   T
 12.3622481474678327  5.1257251772904597 21.1892848364952933   T   T   T
 10.9942904254130589  3.7587925731056941 23.1647190125027365   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_5x2/Pd E_tot= -285.42104026 eV
 D3-zero damping= -10.1108509 eV, D3-BJ damping= -10.7224081 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O
 1.0000000000000000
    13.7399061595000003    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4959624638000006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.9371186129033156
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.4348921796668508  5.4908224917372941  8.9451241821253618   F   F   F
```

1.7174060192708966	2.7428412791459800	8.0000001838787966	F	F	F
3.4348927427375755	3.4071406440833432	8.9451248436730744	F	F	F
1.7174050681011006	0.6591594282543216	8.0000000000000000	F	F	F
1.7174087251004830	5.4908224163631019	11.7805090714841079	F	F	F
3.4348991045795292	2.7428412037717878	10.8353850732375427	F	F	F
1.7174092881712075	3.4071405687091514	11.7805097330318205	F	F	F
3.4348981534097334	0.6591593528801291	10.8353848893587461	F	F	F
3.4350343370134575	5.4040936856420139	14.4187525039209454	T	T	T
1.7172572651244999	2.7173283448554169	13.6695126195374659	T	T	T
3.4349837565508237	3.3890970509171194	14.4723311073185350	T	T	T
1.7169959502904664	0.6571916230082576	13.6735474960105918	T	T	T
1.7177891713919120	5.2286229904815107	16.8259585270563754	T	T	T
3.4350268886779656	2.6648876661862357	16.4632490410535759	T	T	T
1.7171303770635491	3.3562974304809203	17.0970370324471403	T	T	T
3.4350519934250503	0.6122838908988837	16.3904518562348578	T	T	T
6.8698687195418504	5.4908224917372941	8.9451241821253618	F	F	F
5.1523825591458969	2.7428412791459800	8.0000001838787966	F	F	F
6.8698692826125765	3.4071406440833432	8.9451248436730744	F	F	F
5.1523816079761007	0.6591594282543216	8.0000000000000000	F	F	F
5.1523852649754822	5.4908224163631019	11.7805090714841079	F	F	F
6.8698756444545293	2.7428412037717878	10.8353850732375427	F	F	F
5.1523858280462074	3.4071405687091514	11.7805097330318205	F	F	F
6.8698746932847330	0.6591593528801291	10.8353848893587461	F	F	F
6.8700019825508427	5.4041650538213259	14.4184590824922356	T	T	T
5.1527272947236646	2.7173393093671212	13.6695276661793059	T	T	T
6.8699702837031342	3.3890471624508307	14.4725817033956030	T	T	T
5.1530300884216631	0.6572010196980268	13.6735414570522096	T	T	T
5.1522267929990786	5.2285638959579099	16.8259768835916077	T	T	T
6.8700399777027803	2.6636611167766482	16.4634749144531405	T	T	T
5.1529782449566000	3.3562654464449078	17.0969792001834158	T	T	T
6.8700065514730246	0.6115638537396566	16.3903919074813444	T	T	T
10.3048452594168509	5.4908224917372941	8.9451241821253618	F	F	F
8.5873590990208957	2.7428412791459800	8.0000001838787966	F	F	F
10.3048458224875752	3.4071406440833432	8.9451248436730744	F	F	F
8.5873581478511003	0.6591594282543216	8.0000000000000000	F	F	F
8.5873618048504845	5.4908224163631019	11.7805090714841079	F	F	F
10.3048521843295298	2.7428412037717878	10.8353850732375427	F	F	F
8.5873623679212070	3.4071405687091514	11.7805097330318205	F	F	F
10.3048512331597344	0.6591593528801291	10.8353848893587461	F	F	F
10.3049877063125344	5.4040937685768009	14.4187546213607618	T	T	T
8.5872107283806915	2.7173282643798773	13.6695128205625629	T	T	T
10.3049370195095253	3.3890968381103606	14.4723316935415465	T	T	T
8.5869495202881883	0.6571914215931506	13.6735477829937473	T	T	T
8.5877410564292642	5.2286219365240205	16.8259584732914256	T	T	T
10.3049800346009128	2.6648867221240176	16.4632495538014254	T	T	T
8.5870829480466178	3.3562964059924729	17.0970363281888282	T	T	T
10.3050050747200377	0.6122830048001132	16.3904535315473616	T	T	T
13.7398217992918514	5.4908224917372941	8.9451241821253618	F	F	F
12.0223356388958980	2.7428412791459800	8.0000001838787966	F	F	F
13.7398223623625775	3.4071406440833432	8.9451248436730744	F	F	F
12.0223346877261008	0.6591594282543216	8.0000000000000000	F	F	F
12.0223383447254850	5.4908224163631019	11.7805090714841079	F	F	F
13.7398287242045303	2.7428412037717878	10.8353850732375427	F	F	F
12.0223389077962075	3.4071405687091514	11.7805097330318205	F	F	F
13.7398277730347367	0.6591593528801291	10.8353848893587461	F	F	F
13.7399549208430223	5.4041653177992552	14.4184598843578815	T	T	T
12.0226804544303327	2.7173393813122351	13.6695279625072672	T	T	T
13.7399235290528861	3.3890472886375722	14.4725821515243016	T	T	T
12.0229831583052675	0.6572008600844198	13.6735418668697868	T	T	T
12.0221806205708646	5.2285637145339159	16.8259784755752477	T	T	T
13.7399938846958403	2.6636615819392193	16.4634755148571124	T	T	T
12.0229316440543830	3.3562649878836215	17.0969792243270113	T	T	T
13.7399600982495862	0.6115641516903622	16.3903926638024977	T	T	T

```
Metal reference: ZnO(10-10)/fcc(100)_5x2/Pd E_tot= -152.37322306 eV
 D3-zero damping= -10.176678 eV, D3-BJ damping= -12.4345401 eV
Pd
 1.0000000000000000
    13.7399061595000003    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4959624638000006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.8120708806377266
  30
Cartesian
  0.0000020663838809 -0.0000000924696485  7.9452653443765024
  1.3739977577864366  1.3739898780704494  9.9060802658950493
  0.0000024898803304 -0.0000003245314116 11.8668248674547261
  0.0000028172740791  2.7479812975819433  7.9452622470432184
  1.3739980291999931  4.1219725583585651  9.9060802504676193
  0.0000028359274216  2.7479813407270028 11.8668236189231635
  2.7479793017492553 -0.0000003432189375  7.9452402879842632
  4.1219646607103382  1.3739903818997476  9.9060320847345853
  2.7479842349005983 -0.0000005346084910 11.8668162555063681
  2.7479791046148851  2.7479815568341253  7.9452409686302161
  4.1219623564598331  4.1219721021811813  9.9060322591601899
  2.7479843776927555  2.7479817607256143 11.8668159715830175
  5.4959579861508470  0.0000004589581649  7.9452164652113879
  6.8699497889229999  1.3739909352642750  9.9059908460679349
  5.4959611396256056  0.0000007411860433 11.8667808715258367
  5.4959585959933888  2.7479807591629322  7.9452168162618904
  6.8699475539739137  4.1219715588206700  9.9059904642233185
  5.4959608905504655  2.7479805030036055 11.8667799471265258
  8.2439437384688912  0.0000013647083345  7.9452057586395570
  9.6179336096762746  1.3739897640598353  9.9060066278289653
  8.2439436242532249  0.0000018977453472 11.8667605327795638
  8.2439424831628862  2.7479797284247920  7.9452020213240733
  9.6179348987759798  4.1219727446003853  9.9060065463956626
  8.2439438271104155  2.7479795185351445 11.8667624137773746
 10.9919291523034701  0.0000009715612884  7.9452282547814121
 12.3659196173363135  1.3739887701018854  9.9060676041813505
 10.9919210854198592  0.0000012595803518 11.8667913038885455
 10.9919285929724069  2.7479802929092898  7.9452336544455706
 12.3659226165505274  4.1219736312586397  9.9060673097481686
 10.9919209224310261  2.7479799692747231 11.8667865295294295

Interface: ZnO(10-10)/fcc(100)_5x2/Ni E_tot= -444.99955103 eV
 D3-zero damping= -21.2681601 eV, D3-BJ damping= -24.7527213 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Ni
 1.0000000000000000
    12.2692904088500008    0.0000000000000000    0.0000000000000000
     0.0000000000000000    4.9077161635400008    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.1363463028577598
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2  30
Selective dynamics
Cartesian
  3.0672472712836920  4.9031263352545205  8.9451241821253618   F   F   F
  1.5335878539295980  2.4492682707265501  8.0000001838787966   F   F   F
  3.0672477740875803  3.0424660504068544  8.9451248436730744   F   F   F
  1.5335870045658311  0.5886079829877165  8.0000000000000000   F   F   F
  1.5335902701476281  4.9031262679478118 11.7805090714841079   F   F   F
  3.0672534550060346  2.4492682034198419 10.8353850732375427   F   F   F
  1.5335907729515161  3.0424659831001466 11.7805097330318205   F   F   F
  3.0672526056422678  0.5886079156810082 10.8353848893587461   F   F   F
  3.0586869159368595  5.0068527208852167 14.8364397274158648   T   T   T
  1.5294128076866489  2.5348360847857365 13.7231273967150340   T   T   T
```

3.0612986117397911	3.0215516594884693	14.8670406375785529	T	T	T
1.5336456941899239	0.5662906838863249	13.6880067674893233	T	T	T
1.4664116285193216	5.1028481788073794	17.9651115306792946	T	T	T
3.0358436845366308	2.5629997439855923	16.7832229957402959	T	T	T
1.5327583118239825	3.0744327646177960	17.9923246132761925	T	T	T
2.9997589889905161	0.5859289782037674	16.7304905231235921	T	T	T
6.1345698734961918	4.9031263352545205	8.9451241821253618	F	F	F
4.6009104561420990	2.4492682707265501	8.0000001838787966	F	F	F
6.1345703763000810	3.0424660504068544	8.9451248436730744	F	F	F
4.6009096067783313	0.5886079829877165	8.0000000000000000	F	F	F
4.6009128723601274	4.9031262679478118	11.7805090714841079	F	F	F
6.1345760572185348	2.4492682034198419	10.8353850732375427	F	F	F
4.6009133751640157	3.0424659831001466	11.7805097330318205	F	F	F
6.1345752078547680	0.5886079156810082	10.8353848893587461	F	F	F
6.1346685819033304	5.0017511234467431	14.8330640729372210	T	T	T
4.5928770718640681	2.5266216266501660	13.7179536112998139	T	T	T
6.1346077652076891	3.0167880749662048	14.8387870831011828	T	T	T
4.5951706434352309	0.5560260348022181	13.6998248791431330	T	T	T
4.5473052638985330	5.0572980774908105	17.8698583914449678	T	T	T
6.1347409154286909	2.5458824528429247	16.7479984942119238	T	T	T
4.6077855100669636	3.0499817492953731	17.8728984910683373	T	T	T
6.1346822296093668	0.5673840221411872	16.7341945255030105	T	T	T
9.2018924757086911	4.9031263352545205	8.9451241821253618	F	F	F
7.6682330583545983	2.4492682707265501	8.0000001838787966	F	F	F
9.2018929785125803	3.0424660504068544	8.9451248436730744	F	F	F
7.6682322089908306	0.5886079829877165	8.0000000000000000	F	F	F
7.6682354745726293	4.9031262679478118	11.7805090714841079	F	F	F
9.2018986594310341	2.4492682034198419	10.8353850732375427	F	F	F
7.6682359773765159	3.0424659831001466	11.7805097330318205	F	F	F
9.2018978100672690	0.5886079156810082	10.8353848893587461	F	F	F
9.2106332723813154	5.0068569548186375	14.8365979362886122	T	T	T
7.6764300575080222	2.5266357139186240	13.7179632745395175	T	T	T
9.2080290904070736	3.0214831768631893	14.8672557539942503	T	T	T
7.6741810920426587	0.5560496165998721	13.6998599918977195	T	T	T
7.7219082929564191	5.0573261371684195	17.8698734980569647	T	T	T
9.2336048157263999	2.5629585879494998	16.7835346260191010	T	T	T
7.6615872924213679	3.0499833008597741	17.8728537698596632	T	T	T
9.2693915893117023	0.5858787826503780	16.7306854401728380	T	T	T
12.2692150779211921	4.9031263352545205	8.9451241821253618	F	F	F
10.7355556605670994	2.4492682707265501	8.0000001838787966	F	F	F
12.2692155807250831	3.0424660504068544	8.9451248436730744	F	F	F
10.7355548112033325	0.5886079829877165	8.0000000000000000	F	F	F
10.7355580767851304	4.9031262679478118	11.7805090714841079	F	F	F
12.2692212616435352	2.4492682034198419	10.8353850732375427	F	F	F
10.7355585795890178	3.0424659831001466	11.7805097330318205	F	F	F
12.2692204122797701	0.5886079156810082	10.8353848893587461	F	F	F
12.2692867980378661	5.0100294115020931	14.8181160956465927	T	T	T
10.7399337884540085	2.5348815503242208	13.7231061857307992	T	T	T
12.2693066112286591	3.0267170609814680	14.8829937291360679	T	T	T
10.7356346696706151	0.5662832465911491	13.6880191252470258	T	T	T
10.8030558888962762	5.1027566079500639	17.9650250257774360	T	T	T
12.2693253403305356	2.5767752387872895	16.8003803961641438	T	T	T
10.7367424557886295	3.0743952939753814	17.9925891247598599	T	T	T
12.2693302909812836	0.6040950057751528	16.7006692201096918	T	T	T
0.0005002425845740	0.7344878790794522	19.9911914184073218	T	T	T
1.2252872167006734	1.9911470339936621	21.6686370367168877	T	T	T
0.0000359099701591	0.7454601634828071	23.3688225260997129	T	T	T
0.0003040582006748	3.1790720382438753	19.8411115857932572	T	T	T
1.2270718264742591	4.4003823069263879	21.6671228175091315	T	T	T
0.0001824457328801	3.1954863575037327	23.4094972270920678	T	T	T
2.5130104498809924	0.7509336454792668	20.0544614013929312	T	T	T
3.6773989628972581	2.0248526897115759	21.7080643201827534	T	T	T
2.4443671255465693	0.7504405235807161	23.3787879851228091	T	T	T

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  2.4060574067357550  3.1860217355056140 19.8156399833736891   T   T   T
  3.6798327145293017  4.3878095394088703 21.6942761049038388   T   T   T
  2.4342461656814289  3.2070584265644992 23.4314865613882013   T   T   T
  4.9342646538103860  0.7655815436096293 20.1296558506685912   T   T   T
  6.1347193469323251  2.0430794148230138 21.7272775923685835   T   T   T
  4.9031473220047515  0.7567438061751860 23.3913879265242386   T   T   T
  4.8717394174758519  3.1897453213954394 19.8008180293160336   T   T   T
  6.1344011854074214  4.3830948289902212 21.7078162953513036   T   T   T
  4.8951705345855965  3.2172557681633851 23.4641496146973445   T   T   T
  7.3357701082704301  0.7655502535851454 20.1299373975501332   T   T   T
  8.5920713070955728  2.0248982944685068 21.7081561558089291   T   T   T
  7.3658763047469948  0.7565914121866594 23.3913744081786206   T   T   T
  7.3975948620043530  3.1893137992920741 19.8005078647180781   T   T   T
  8.5899578597179449  4.3876206332954508 21.6948663219322881   T   T   T
  7.3745228708320321  3.2169458200895402 23.4644450520115377   T   T   T
  9.7565321722337419  0.7510022723874706 20.0546381200380033   T   T   T
 11.0442495917146761  1.9906930489075989 21.6686324834637176   T   T   T
  9.8254437383718773  0.7499962805692747 23.3785672735153156   T   T   T
  9.8632467502252918  3.1860549706342161 19.8159131527698094   T   T   T
 11.0428499464742753  4.3997855925070537 21.6669427036760354   T   T   T
  9.8356356464910313  3.2068888928958983 23.4318707759239153   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_5x2/Ni E_tot= -281.82672126 eV
 D3-zero damping= -11.228546 eV, D3-BJ damping= -12.7454453 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O
 1.0000000000000000
    12.2692904088500008    0.0000000000000000    0.0000000000000000
     0.0000000000000000    4.9077161635400008    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.9371186129033156
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.0672472712836920  4.9031263352545205  8.9451241821253618   F   F   F
  1.5335878539295980  2.4492682707265501  8.0000001838787966   F   F   F
  3.0672477740875803  3.0424660504068544  8.9451248436730744   F   F   F
  1.5335870045658311  0.5886079829877165  8.0000000000000000   F   F   F
  1.5335902701476281  4.9031262679478118 11.7805090714841079   F   F   F
  3.0672534550060346  2.4492682034198419 10.8353850732375427   F   F   F
  1.5335907729515161  3.0424659831001466 11.7805097330318205   F   F   F
  3.0672526056422678  0.5886079156810082 10.8353848893587461   F   F   F
  3.0673908283247369  4.9890402336585939 14.7979487775911860   T   T   T
  1.5328812789581561  2.5434041585670171 13.7339842836236201   T   T   T
  3.0673107758773583  3.0125417640062788 14.8775354784930212   T   T   T
  1.5331540459935435  0.5711231826492825 13.6894228302379215   T   T   T
  1.5343006755979243  4.7882580498671690 17.6553233217378214   T   T   T
  3.0674612966621471  2.5434517415257951 16.8442032805511488   T   T   T
  1.5347408993116398  2.9515479069044921 17.9752164791820448   T   T   T
  3.0675803439777987  0.5828085396940271 16.7200315969775026   T   T   T
  6.1345698734961918  4.9031263352545205  8.9451241821253618   F   F   F
  4.6009104561420990  2.4492682707265501  8.0000001838787966   F   F   F
  6.1345703763000810  3.0424660504068544  8.9451248436730744   F   F   F
  4.6009096067783313  0.5886079829877165  8.0000000000000000   F   F   F
  4.6009128723601274  4.9031262679478118 11.7805090714841079   F   F   F
  6.1345760572185348  2.4492682034198419 10.8353850732375427   F   F   F
  4.6009133751640157  3.0424659831001466 11.7805097330318205   F   F   F
  6.1345752078547680  0.5886079156810082 10.8353848893587461   F   F   F
  6.1345566274473153  4.9889046688528520 14.7997351943715625   T   T   T
  4.6016882948986577  2.5436185702226055 13.7338758545327746   T   T   T
  6.1345622160592459  3.0125375301962340 14.8798064052773000   T   T   T
  4.6015197733904714  0.5713405369757869 13.6892751486807107   T   T   T
  4.6005509011965158  4.7882989934789864 17.6559375701599812   T   T   T
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  6.1346241417305469  2.5434309836084315 16.8476497564890053   T   T   T
  4.6000213335470317  2.9515479905016377 17.9754981651557131   T   T   T
  6.1346005408328805  0.5827974892592062 16.7218984400660311   T   T   T
  9.2018924757086911  4.9031263352545205  8.9451241821253618   F   F   F
  7.6682330583545983  2.4492682707265501  8.0000001838787966   F   F   F
  9.2018929785125803  3.0424660504068544  8.9451248436730744   F   F   F
  7.6682322089908306  0.5886079829877165  8.0000000000000000   F   F   F
  7.6682354745726293  4.9031262679478118 11.7805090714841079   F   F   F
  9.2018986594310341  2.4492682034198419 10.8353850732375427   F   F   F
  7.6682359773765159  3.0424659831001466 11.7805097330318205   F   F   F
  9.2018978100672690  0.5886079156810082 10.8353848893587461   F   F   F
  9.2020474706061783  4.9890424806977771 14.7979412415694647   T   T   T
  7.6675077686936435  2.5434350670611106 13.7339876973632933   T   T   T
  9.2019506120350183  3.0125512511640133 14.8775374318119518   T   T   T
  7.6677920835599176  0.5711485614539127 13.6894218913419685   T   T   T
  7.6689359303487477  4.7882983623647579 17.6553477802635541   T   T   T
  9.2020912072949965  2.5434583333607650 16.8442047881843173   T   T   T
  7.6693781634367477  2.9515778626003009 17.9752124909696249   T   T   T
  9.2022191517286629  0.5828145754258137 16.7200355487182222   T   T   T
 12.2692150779211921  4.9031263352545205  8.9451241821253618   F   F   F
 10.7355556605670994  2.4492682707265501  8.0000001838787966   F   F   F
 12.2692155807250831  3.0424660504068544  8.9451248436730744   F   F   F
 10.7355548112033325  0.5886079829877165  8.0000000000000000   F   F   F
 10.7355580767851304  4.9031262679478118 11.7805090714841079   F   F   F
 12.2692212616435352  2.4492682034198419 10.8353850732375427   F   F   F
 10.7355585795890178  3.0424659831001466 11.7805097330318205   F   F   F
 12.2692204122797701  0.5886079156810082 10.8353848893587461   F   F   F
 12.2692039248031968  4.9888715582129910 14.7997254111693035   T   T   T
 10.7363396512411153  2.5436138119405656 13.7338935841643472   T   T   T
 12.2692310185969831  3.0125154138045742 14.8798140325552968   T   T   T
 10.7361633539665391  0.5713377556486625 13.6892794870103600   T   T   T
 10.7351918964302051  4.7882670290180114 17.6559011730234552   T   T   T
 12.2692699455793637  2.5433988873775601 16.8476659715026855   T   T   T
 10.7346643293661099  2.9515232850095945 17.9754904967408535   T   T   T
 12.2692489510506881  0.5827717502481832 16.7218942484011350   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_5x2/Ni E_tot= -154.0709124 eV
 D3-zero damping= -6.7890372 eV, D3-BJ damping= -8.7776248 eV
Ni
 1.0000000000000000
    12.2692904088500008    0.0000000000000000    0.0000000000000000
     0.0000000000000000    4.9077161635400008    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.8120708806377266
  30
Cartesian
 -0.0000024823048820  0.0000028189801951  8.1769172905703016
  1.2269042804926391  1.2269317459946611  9.9060234746400617
 -0.0000011463076574  0.0000025542059238 11.6348959909609917
 -0.0000025768643288  2.4538609103302433  8.1769134305022320
  1.2269051334432153  3.6807902112645206  9.9060228242081898
 -0.0000004691667242  2.4538609974511214 11.6348895091098470
  2.4538509999406011  0.0000030492550796  8.1771930037636675
  3.6807854189447315  1.2269376864435186  9.9060198641202533
  2.4538569888659056  0.0000030691754967 11.6348795896116517
  2.4538504724747723  2.4538605629871375  8.1771913793950457
  3.6807878835561616  3.6807794576746637  9.9060247919195294
  2.4538627641860078  2.4538613606935438 11.6348833885846741
  4.9077131803556249  0.0000024753926146  8.1771627480293922
  6.1346637411266443  1.2269347875391523  9.9060043495108445
  4.9077150183390437 -0.0000116849439558 11.6348312448976756
  4.9077122123493337  2.4538614011485391  8.1771646495000585
  6.1346595709855922  3.6807823797980475  9.9060113494715942
  4.9077767244090156  2.4537978458865219 11.6349830637549942
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  7.3615711013574829  0.0000024692610512  8.1771471194817504
  8.5884724500381289  1.2269309357426836  9.9060115268394373
  7.3615689291885413  0.0000036925437937 11.6351133161716778
  7.3615717584204372  2.4538608427315296  8.1771423639181720
  8.5884724822715945  3.6807910808074973  9.9060120092321355
  7.3615782427728398  2.4538613082219354 11.6351134368250797
  9.8154344316001687  0.0000030349357709  8.1771803211104714
 11.0423900801480563  1.2269307759645864  9.9060068720270671
  9.8154258138189583  0.0000031004916896 11.6348390062534435
  9.8154333549737682  2.4538608288366306  8.1771880779821835
 11.0423913098519471  3.6807912322126710  9.9060066475430908
  9.8154276138963645  2.4538606630916449 11.6348356750618969

Interface: ZnO(10-10)/fcc(100)_5x2/Ir E_tot= -548.94856583 eV
 D3-zero damping= -27.8812582 eV, D3-BJ damping= -28.4180783 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Ir
 1.0000000000000000
    13.5753160727500024    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4301264291000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.1824709295180504
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2  30
Selective dynamics
Cartesian
  3.3937456685287555  5.4250480286694351  8.9451241821253618   F   F   F
  1.6968332437063909  2.7099848331968222  8.0000001838787966   F   F   F
  3.3937462248544659  3.3663265680868064  8.9451248436730744   F   F   F
  1.6968323039306406  0.6512633694152701  8.0000000000000000   F   F   F
  1.6968359171228937  5.4250479541981491 11.7805090714841079   F   F   F
  3.3937525104880302  2.7099847587255361 10.8353850732375427   F   F   F
  1.6968364734486043  3.3663264936155204 11.7805097330318205   F   F   F
  3.3937515707122801  0.6512632949439837 10.8353848893587461   F   F   F
  3.3684355165749569  5.3853753386142724 14.4633386361121072   T   T   T
  1.6678363583379427  2.7082828294611656 13.6947405288497723   T   T   T
  3.3925028536035993  3.3740710994923049 14.5340007532753113   T   T   T
  1.6791075632296351  0.6768032267739854 13.6524370999233913   T   T   T
  1.6544920166318529  5.6111078221884876 17.2791241535893398   T   T   T
  3.4412310458315556  2.7041411498183519 16.4452550010369762   T   T   T
  1.8431243338749217  3.5573227211153622 17.3149938885949410   T   T   T
  3.3716739697700846  0.7190471915366605 16.3094051030781131   T   T   T
  6.7875746867162556  5.4250480286694351  8.9451241821253618   F   F   F
  5.0906622618938924  2.7099848331968222  8.0000001838787966   F   F   F
  6.7875752430419674  3.3663265680868064  8.9451248436730744   F   F   F
  5.0906613221181418  0.6512633694152701  8.0000000000000000   F   F   F
  5.0906649353103939  5.4250479541981491 11.7805090714841079   F   F   F
  6.7875815286755312  2.7099847587255361 10.8353850732375427   F   F   F
  5.0906654916361047  3.3663264936155204 11.7805097330318205   F   F   F
  6.7875805888997807  0.6512632949439837 10.8353848893587461   F   F   F
  6.7874966046612526  5.3594300865256654 14.4233856425234546   T   T   T
  5.0788254711984830  2.6765569663379205 13.6518931666276799   T   T   T
  6.7875262587667073  3.3537979586886446 14.4926976239269987   T   T   T
  5.0759122577660403  0.6541028906946497 13.6541954386276316   T   T   T
  5.0720024421783751  5.5038147267128563 17.1306081467824320   T   T   T
  6.7874774460644076  2.6500084763804668 16.3897265763281652   T   T   T
  5.1595326562726331  3.4731783030573937 17.1955621729547445   T   T   T
  6.7875206616355799  0.6769483151447033 16.2694917075422829   T   T   T
 10.1814037049037562  5.4250480286694351  8.9451241821253618   F   F   F
  8.4844912800813912  2.7099848331968222  8.0000001838787966   F   F   F
 10.1814042612294671  3.3663265680868064  8.9451248436730744   F   F   F
  8.4844903403056406  0.6512633694152701  8.0000000000000000   F   F   F
  8.4844939534978963  5.4250479541981491 11.7805090714841079   F   F   F
 10.1814105468630309  2.7099847587255361 10.8353850732375427   F   F   F
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  8.4844945098236053  3.3663264936155204 11.7805097330318205   F   F   F
 10.1814096070872839  0.6512632949439837 10.8353848893587461   F   F   F
 10.2067087983895188  5.3853457698203249 14.4633768418301543   T   T   T
  8.4962529504564870  2.6765278174548084 13.6518943649318203   T   T   T
 10.1825082264946847  3.3740478133410687 14.5340351963017280   T   T   T
  8.4991287752090781  0.6540605839279034 13.6542145235328398   T   T   T
  8.5030255141678079  5.5038380860941274 17.1305940841229827   T   T   T
 10.1339211526917765  2.7040438334339827 16.4453212830562059   T   T   T
  8.4155162888759634  3.4731672729699818 17.1955303475489210   T   T   T
 10.2034602540267070  0.7190118970356388 16.3094314862141161   T   T   T
 13.5752327230912577  5.4250480286694351  8.9451241821253618   F   F   F
 11.8783202982688927  2.7099848331968222  8.0000001838787966   F   F   F
 13.5752332794169703  3.3663265680868064  8.9451248436730744   F   F   F
 11.8783193584931439  0.6512633694152701  8.0000000000000000   F   F   F
 11.8783229716853977  5.4250479541981491 11.7805090714841079   F   F   F
 13.5752395650505342  2.7099847587255361 10.8353850732375427   F   F   F
 11.8783235280111068  3.3663264936155204 11.7805097330318205   F   F   F
 13.5752386252747854  0.6512632949439837 10.8353848893587461   F   F   F
 13.5751081874508532  5.4074381892098078 14.4973837330682116   T   T   T
 11.9070496622142965  2.7082474043624760 13.6946910621957052   T   T   T
 13.5751104054060807  3.3925440701924803 14.6692381763680242   T   T   T
 11.8958442250124872  0.6768034091683375 13.6524233614375223   T   T   T
 11.9206152244000467  5.6110513212721767 17.2791484725901121   T   T   T
 13.5751140793152789  2.7952132916352697 16.6530526994098445   T   T   T
 11.7319132077567119  3.5573351205211381 17.3149804839744270   T   T   T
 13.5752050838717508  0.7882210131137048 16.3280021245425573   T   T   T
 -0.0001133483373087  0.9002483299967027 19.4449040267973388   T   T   T
  1.3708569284276793  2.2632035978492668 21.3166675454490040   T   T   T
 -0.0001067182042315  0.9051856874454852 23.1461309606069356   T   T   T
 -0.0001102619177183  3.6063687862753380 19.4927074076280284   T   T   T
  1.3704948838057254  4.9714811917954203 21.3165197448750376   T   T   T
 -0.0001019846894291  3.6180567741751801 23.1638513314777548   T   T   T
  2.7157120295069901  0.9138389757186920 19.4722787711189547   T   T   T
  4.0812017683978103  2.2953176568338138 21.2614283237561672   T   T   T
  2.7428368502051006  0.9061416754260301 23.1362976152025333   T   T   T
  2.6582248690316748  3.6071429657831144 19.3632805473053544   T   T   T
  4.0791309439210517  4.9508381506885870 21.2446070981377844   T   T   T
  2.7343913623051490  3.6255727468445587 23.1483181372861502   T   T   T
  5.4278362514582499  0.9187901567407339 19.4637299295047903   T   T   T
  6.7875360464199490  2.3066241401824050 21.2422866696235211   T   T   T
  5.4414305707164239  0.9082390678910073 23.0995879273414140   T   T   T
  5.3979081936314675  3.6102485167847429 19.3003477512205848   T   T   T
  6.7875404655852583  4.9440663370227300 21.2163679245162164   T   T   T
  5.4369932568065549  3.6370336431614256 23.1320175659836949   T   T   T
  8.1472293749496245  0.9187826183344346 19.4637454827637448   T   T   T
  9.4938517232194641  2.2953000302502926 21.2614285671556473   T   T   T
  8.1336175664015400  0.9082420318583784 23.0996082026463476   T   T   T
  8.1771993028767795  3.6102365322052958 19.3003276522841993   T   T   T
  9.4959510809009977  4.9508277404501007 21.2446176571464527   T   T   T
  8.1380926075795568  3.6370352156796746 23.1320211616846763   T   T   T
 10.8593667141199841  0.9138349158812379 19.4722953426413241   T   T   T
 12.2042489812691120  2.2632099991184211 21.3166695305563536   T   T   T
 10.8322633058027762  0.9061383683944002 23.1363056949702646   T   T   T
 10.9168200797882697  3.6071296439076783 19.3633190808384832   T   T   T
 12.2046046111439281  4.9714737704975880 21.3165247056796758   T   T   T
 10.8406998730443771  3.6255723318796931 23.1483211010226668   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_5x2/Ir E_tot= -286.520623 eV
 D3-zero damping= -10.1978153 eV, D3-BJ damping= -10.9213331 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O
 1.0000000000000000
    13.5753160727500024    0.0000000000000000    0.0000000000000000
```

```
     0.0000000000000000    5.4301264291000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.9371186129033156
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.3937456685287555  5.4250480286694351  8.9451241821253618   F   F   F
  1.6968332437063909  2.7099848331968222  8.0000001838787966   F   F   F
  3.3937462248544659  3.3663265680868064  8.9451248436730744   F   F   F
  1.6968323039306406  0.6512633694152701  8.0000000000000000   F   F   F
  1.6968359171228937  5.4250479541981491 11.7805090714841079   F   F   F
  3.3937525104880302  2.7099847587255361 10.8353850732375427   F   F   F
  1.6968364734486043  3.3663264936155204 11.7805097330318205   F   F   F
  3.3937515707122801  0.6512632949439837 10.8353848893587461   F   F   F
  3.3937741837763840  5.3523023853239682 14.4559521628160823   T   T   T
  1.6959035499257440  2.6915406492579197 13.6771002124852590   T   T   T
  3.3938005569585274  3.3462512401957527 14.5150994710737891   T   T   T
  1.6960696348930266  0.6492958184637950 13.6763877311428548   T   T   T
  1.6975734037740182  5.1687140710717712 16.9041359075899571   T   T   T
  3.3938699479803880  2.6411505499611354 16.5044535168624869   T   T   T
  1.6970479867816561  3.3078266662000408 17.1947726930455822   T   T   T
  3.3938095114985436  0.6073467828618315 16.4234693554713935   T   T   T
  6.7875746867162556  5.4250480286694351  8.9451241821253618   F   F   F
  5.0906622618938924  2.7099848331968222  8.0000001838787966   F   F   F
  6.7875752430419674  3.3663265680868064  8.9451248436730744   F   F   F
  5.0906613221181418  0.6512633694152701  8.0000000000000000   F   F   F
  5.0906649353103939  5.4250479541981491 11.7805090714841079   F   F   F
  6.7875815286755312  2.7099847587255361 10.8353850732375427   F   F   F
  5.0906654916361047  3.3663264936155204 11.7805097330318205   F   F   F
  6.7875805888997807  0.6512632949439837 10.8353848893587461   F   F   F
  6.7875618246336824  5.3561082354169907 14.4605732732682135   T   T   T
  5.0916764885371686  2.6915894596524583 13.6770841048765615   T   T   T
  6.7876098397339826  3.3483687917962288 14.5167115710848424   T   T   T
  5.0914348716415825  0.6493141201712043 13.6763754552586345   T   T   T
  5.0900879602869971  5.1687875360696394 16.9041145446278378   T   T   T
  6.7876190514496999  2.6432058850401172 16.5064820194404973   T   T   T
  5.0906016845839774  3.3078556932954060 17.1947942948863393   T   T   T
  6.7876449360168358  0.6076654402452711 16.4263524721622360   T   T   T
 10.1814037049037562  5.4250480286694351  8.9451241821253618   F   F   F
  8.4844912800813912  2.7099848331968222  8.0000001838787966   F   F   F
 10.1814042612294671  3.3663265680868064  8.9451248436730744   F   F   F
  8.4844903403056406  0.6512633694152701  8.0000000000000000   F   F   F
  8.4844939534978963  5.4250479541981491 11.7805090714841079   F   F   F
 10.1814105468630309  2.7099847587255361 10.8353850732375427   F   F   F
  8.4844945098236053  3.3663264936155204 11.7805097330318205   F   F   F
 10.1814096070872839  0.6512632949439837 10.8353848893587461   F   F   F
 10.1814230399554884  5.3523029614943427 14.4559670271461460   T   T   T
  8.4835576106197905  2.6915411782947154 13.6771034649301377   T   T   T
 10.1814579166822554  3.3462513915550529 14.5150987001822678   T   T   T
  8.4837269792213181  0.6492964337727549 13.6763879411124130   T   T   T
  8.4851922729322666  5.1687205853870539 16.9041386755786078   T   T   T
 10.1815253039961249  2.6411616961750095 16.5044568522748456   T   T   T
  8.4846898359278882  3.3078250247580216 17.1947774085882870   T   T   T
 10.1814620397459947  0.6073506296266893 16.4234811012611885   T   T   T
 13.5752327230912577  5.4250480286694351  8.9451241821253618   F   F   F
 11.8783202982688927  2.7099848331968222  8.0000001838787966   F   F   F
 13.5752332794169703  3.3663265680868064  8.9451248436730744   F   F   F
 11.8783193584931439  0.6512633694152701  8.0000000000000000   F   F   F
 11.8783229716853977  5.4250479541981491 11.7805090714841079   F   F   F
 13.5752395650505342  2.7099847587255361 10.8353850732375427   F   F   F
 11.8783235280111068  3.3663264936155204 11.7805097330318205   F   F   F
 13.5752386252747854  0.6512632949439837 10.8353848893587461   F   F   F
 13.5752099171038108  5.3561107991295245 14.4605588469552497   T   T   T
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 11.8793320625598113  2.6915886966614613 13.6770839345429778   T   T   T
 13.5752703756947266  3.3483704400334759 14.5167013301304433   T   T   T
 11.8790822935021385  0.6493143552141649 13.6763743000409068   T   T   T
 11.8777439173200392  5.1687827706658842 16.9041154782381611   T   T   T
 13.5753253629641293  2.6432066548353306 16.5064309373722296   T   T   T
 11.8782821412026323  3.3078468201224038 17.1947779872435156   T   T   T
 13.5753047105873392  0.6076610694392355 16.4263348197883872   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_5x2/Ir E_tot= -251.82818206 eV
 D3-zero damping= -12.40592 eV, D3-BJ damping= -13.446679 eV
Ir
 1.0000000000000000
    13.5753160727500024    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4301264291000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.8120708806377266
  30
Cartesian
  0.0000023914793500 -0.0000000952101374  8.0527847852028778
  1.3575342616198258  1.3575310846356301  9.9060520341892300
 -0.0000000050602074 -0.0000001929077197 11.7592826630993592
  0.0000023218097561  2.7150632975790407  8.0527866786703530
  1.3575351622643037  4.0725952738799496  9.9060518694234947
 -0.0000001293854082  2.7150633152325256 11.7592822030041653
  2.7150583915421076  0.0000004337853528  8.0527772110819491
  4.0725924188950433  1.3575317470230683  9.9060250701118395
  2.7150683269214069  0.0000003021469052 11.7592792635443715
  2.7150582014592679  2.7150627331417923  8.0527769905448583
  4.0725900273672275  4.0725946878291950  9.9060250654709776
  2.7150685244779900  2.7150629066894938 11.7592792169535194
  5.4301209010915352  0.0000000171787327  8.0527581626080575
  6.7876569060523249  1.3575315586087455  9.9060009466835357
  5.4301295988881950  0.0000001937589365 11.7592556308555700
  5.4301208667157708  2.7150631949190087  8.0527576144428643
  6.7876552109113870  4.0725949004134181  9.9060011531967884
  5.4301293600560863  2.7150630329334939 11.7592562265092919
  8.1451903906918339  0.0000002379682205  8.0527506318887614
  9.5027206185136031  1.3575313618690756  9.9060105941391221
  8.1451879945125079  0.0000005987881875 11.7592488136860691
  8.1451903923873328  2.7150629268613065  8.0527523531119254
  9.5027218132698419  4.0725951115537713  9.9060106634726459
  8.1451882850885671  2.7150627075457709 11.7592474992705363
 10.8602600045130373  0.0000003976732832  8.0527689248087118
 12.2177859199630312  1.3575310441741777  9.9060443167378747
 10.8602463570859928  0.0000005214053539 11.7592643482758632
 10.8602600686707902  2.7150628193289759  8.0527675639325587
 12.2177878788858418  4.0725953281740495  9.9060441998954527
 10.8602463009132961  2.7150627044219160 11.7592655425895600

Interface: ZnO(10-10)/fcc(100)_5x2/Rh E_tot= -504.81324307 eV
 D3-zero damping= -25.5799357 eV, D3-BJ damping= -27.1004706 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Rh
 1.0000000000000000
    13.3883134764000005    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3553253905600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.1824709295180504
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2  30
Selective dynamics
Cartesian
  3.3469961675988746  5.3503169460745283  8.9451241821253618   F   F   F
  1.6734590386090200  2.6726542696091213  8.0000001838787966   F   F   F
  3.3469967162610916  3.3199547705521724  8.9451248436730744   F   F   F
```

1.6734581117788621	0.6422920909319076	8.0000000000000000	F	F	F
1.6734616751986953	5.3503168726290991	11.7805090714841079	F	F	F
3.3470029153088414	2.6726541961636912	10.8353850732375427	F	F	F
1.6734622238609118	3.3199546971067431	11.7805097330318205	F	F	F
3.3470019884786835	0.6422920174864777	10.8353848893587461	F	F	F
3.3258839313727542	5.3108950725518804	14.5157910081128723	T	T	T
1.6566490623857488	2.6699546623651615	13.6896926310496383	T	T	T
3.3420194395226175	3.3086357588742970	14.5853298097515260	T	T	T
1.6616032847154709	0.6529705679598876	13.6612875992924039	T	T	T
1.6223434761534432	5.4602242416284463	17.3597557698626872	T	T	T
3.3607391860877973	2.6544002962196891	16.5071436240662877	T	T	T
1.7369192900236874	3.4401286203844497	17.3710356142901361	T	T	T
3.3099456541779886	0.6715920730290073	16.3854917315415065	T	T	T
6.6940745366988743	5.3503169460745283	8.9451241821253618	F	F	F
5.0205374077090212	2.6726542696091213	8.0000001838787966	F	F	F
6.6940750853610922	3.3199547705521724	8.9451248436730744	F	F	F
5.0205364808788628	0.6422920909319076	8.0000000000000000	F	F	F
5.0205400442986949	5.3503168726290991	11.7805090714841079	F	F	F
6.6940812844088411	2.6726541961636912	10.8353850732375427	F	F	F
5.0205405929609119	3.3199546971067431	11.7805097330318205	F	F	F
6.6940803575786836	0.6422920174864777	10.8353848893587461	F	F	F
6.6928949751860163	5.2905929620471817	14.4917780846874109	T	T	T
5.0079870143617979	2.6487738953858742	13.6669981781705143	T	T	T
6.6932964097005927	3.2918055895994534	14.5456463744245319	T	T	T
5.0082444792635963	0.6339255144540991	13.6684438166840092	T	T	T
4.9844309113094631	5.3801488269458897	17.2278896584046350	T	T	T
6.6930891646920649	2.6075669493225115	16.4554008880015203	T	T	T
5.0601810001128804	3.3778412255446884	17.2581469385328248	T	T	T
6.6923703788447337	0.6332252494441395	16.3665561385728253	T	T	T
10.0411529057988744	5.3503169460745283	8.9451241821253618	F	F	F
8.3676157768090196	2.6726542696091213	8.0000001838787966	F	F	F
10.0411534544610923	3.3199547705521724	8.9451248436730744	F	F	F
8.3676148499788621	0.6422920909319076	8.0000000000000000	F	F	F
8.3676184133986968	5.3503168726290991	11.7805090714841079	F	F	F
10.0411596535088421	2.6726541961636912	10.8353850732375427	F	F	F
8.3676189620609112	3.3199546971067431	11.7805097330318205	F	F	F
10.0411587266786846	0.6422920174864777	10.8353848893587461	F	F	F
10.0601837032544097	5.3103114926548827	14.5155364906210966	T	T	T
8.3785531577681169	2.6482472271597404	13.6666747093758421	T	T	T
10.0445775607133676	3.3082019581697137	14.5838736301686787	T	T	T
8.3777049543623328	0.6336164389076656	13.6685419417262537	T	T	T
8.4005852843933404	5.3800562427704737	17.2263204057141124	T	T	T
10.0251260201803731	2.6533031348239264	16.5051887472121379	T	T	T
8.3266651876105708	3.3776334864390170	17.2567579478561939	T	T	T
10.0760417449009427	0.6707024361072971	16.3852139342047742	T	T	T
13.3882312748988763	5.3503169460745283	8.9451241821253618	F	F	F
11.7146941459090215	2.6726542696091213	8.0000001838787966	F	F	F
13.3882318235610942	3.3199547705521724	8.9451248436730744	F	F	F
11.7146932190788640	0.6422920909319076	8.0000000000000000	F	F	F
11.7146967824986987	5.3503168726290991	11.7805090714841079	F	F	F
13.3882380226088422	2.6726541961636912	10.8353850732375427	F	F	F
11.7146973311609131	3.3199546971067431	11.7805097330318205	F	F	F
13.3882370957786865	0.6422920174864777	10.8353848893587461	F	F	F
13.3873221496868329	5.3286680189075870	14.5296429079848455	T	T	T
11.7304508348838699	2.6697639679990877	13.6895127744680387	T	T	T
13.3876545662905588	3.3244037493203087	14.6528304799473386	T	T	T
11.7246627263362466	0.6527401965150688	13.6613637151597693	T	T	T
11.7649446087415335	5.4589465716781698	17.3580851697801890	T	T	T
13.3875197635742538	2.7160310236100220	16.6043254082064280	T	T	T
11.6484236133000874	3.4392156005198404	17.3675310448035809	T	T	T
13.3876394366572491	0.7239577604847168	16.3826684747746079	T	T	T
0.0041002394840831	0.9257103082743797	19.4606105799246336	T	T	T
1.3531362080101510	2.2648811232832520	21.3093135274286993	T	T	T

```
  0.0037778410771365  0.9183274332069414 23.1189448761900493   T   T   T
  0.0046364227620311  3.5918901766430040 19.4797771156308492   T   T   T
  1.3526006271814517  4.9325782121785151 21.3007029392090530   T   T   T
  0.0040808321965582  3.5991152677527460 23.1429220154899618   T   T   T
  2.7058760756621347  0.9428892726957279 19.4990632879784158   T   T   T
  4.0292013340387163  2.2958566970998540 21.3021327183499274   T   T   T
  2.6921557020439031  0.9206789493436855 23.1237369867910125   T   T   T
  2.6503690357974521  3.5882229732281550 19.3909790779433315   T   T   T
  4.0268518627818022  4.9210556962169889 21.2644762141542749   T   T   T
  2.6856886414722942  3.6117401437467311 23.1435402302807063   T   T   T
  5.3710094692263457  0.9550787412674605 19.5217363607943355   T   T   T
  6.6989679009648091  2.3107082539912192 21.3060742750751260   T   T   T
  5.3651902550889456  0.9280210925600579 23.1216265335674969   T   T   T
  5.3380551560448088  3.5903695453968925 19.3495173074771927   T   T   T
  6.6986695999111152  4.9133074186247336 21.2544478251634814   T   T   T
  5.3568061698137717  3.6308148627913019 23.1521077290274455   T   T   T
  8.0245226200362509  0.9542884898987847 19.5207362153166457   T   T   T
  9.3683258673920555  2.2958104124714591 21.2996455945999088   T   T   T
  8.0338237767964618  0.9270289481685213 23.1211341345806041   T   T   T
  8.0563429695040671  3.5905795825651459 19.3478988289592522   T   T   T
  9.3701187947380031  4.9203046931753578 21.2635976065363934   T   T   T
  8.0383574979917309  3.6299492691959205 23.1519484787401417   T   T   T
 10.6899362812355818  0.9424534129793798 19.4980601503407982   T   T   T
 12.0441767069283436  2.2656426883137448 21.3080693146423918   T   T   T
 10.7065822021352091  0.9199679346134854 23.1216481145674280   T   T   T
 10.7456977974432544  3.5877255499111236 19.3879070532373525   T   T   T
 12.0444240308088570  4.9325144726905688 21.2985120801261409   T   T   T
 10.7106237160527904  3.6108742340977358 23.1429801249938016   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_5x2/Rh E_tot= -287.38810715 eV
 D3-zero damping= -10.302526 eV, D3-BJ damping= -11.1531535 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O
 1.0000000000000000
    13.3883134764000005    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3553253905600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.9371186129033156
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.3469961675988746  5.3503169460745283  8.9451241821253618   F   F   F
  1.6734590386090200  2.6726542696091213  8.0000001838787966   F   F   F
  3.3469967162610916  3.3199547705521724  8.9451248436730744   F   F   F
  1.6734581117788621  0.6422920909319076  8.0000000000000000   F   F   F
  1.6734616751986953  5.3503168726290991 11.7805090714841079   F   F   F
  3.3470029153088414  2.6726541961636912 10.8353850732375427   F   F   F
  1.6734622238609118  3.3199546971067431 11.7805097330318205   F   F   F
  3.3470019884786835  0.6422920174864777 10.8353848893587461   F   F   F
  3.3470664503649581  5.2906618630011346 14.4983886304325758   T   T   T
  1.6738125987206636  2.6637046831478837 13.6865507431628117   T   T   T
  3.3470827630953925  3.2944540698896594 14.5695092212817787   T   T   T
  1.6732836641602600  0.6375158343333448 13.6778120072034035   T   T   T
  1.6732532557494146  5.0996638995941934 16.9938466339698024   T   T   T
  3.3471394734212456  2.6133784204318671 16.5631057347565545   T   T   T
  1.6731132592967759  3.2507791291537833 17.3121359760855498   T   T   T
  3.3470934552951439  0.5987497817269934 16.4595488452770198   T   T   T
  6.6940745366988743  5.3503169460745283  8.9451241821253618   F   F   F
  5.0205374077090212  2.6726542696091213  8.0000001838787966   F   F   F
  6.6940750853610922  3.3199547705521724  8.9451248436730744   F   F   F
  5.0205364808788628  0.6422920909319076  8.0000000000000000   F   F   F
  5.0205400442986949  5.3503168726290991 11.7805090714841079   F   F   F
  6.6940812844088411  2.6726541961636912 10.8353850732375427   F   F   F
```

```
  5.0205405929609119  3.3199546971067431 11.7805097330318205   F   F   F
  6.6940803575786836  0.6422920174864777 10.8353848893587461   F   F   F
  6.6941603627875335  5.2921431397997694 14.4996072873626982   T   T   T
  5.0203354942320777  2.6636719827721542 13.6865291694288196   T   T   T
  6.6941422147375471  3.2953403844996894 14.5683463905009702   T   T   T
  5.0208605089221576  0.6374980994460944 13.6778218368922406   T   T   T
  5.0209662588816331  5.0997207679412844 16.9938280646220399   T   T   T
  6.6941638158366263  2.6145483983374014 16.5607150329298953   T   T   T
  5.0211283798143551  3.2508252321643387 17.3121443993798039   T   T   T
  6.6941832684390494  0.5994208031617514 16.4599644861636811   T   T   T
 10.0411529057988744  5.3503169460745283  8.9451241821253618   F   F   F
  8.3676157768090196  2.6726542696091213  8.0000001838787966   F   F   F
 10.0411534544610923  3.3199547705521724  8.9451248436730744   F   F   F
  8.3676148499788621  0.6422920909319076  8.0000000000000000   F   F   F
  8.3676184133986968  5.3503168726290991 11.7805090714841079   F   F   F
 10.0411596535088421  2.6726541961636912 10.8353850732375427   F   F   F
  8.3676189620609112  3.3199546971067431 11.7805097330318205   F   F   F
 10.0411587266786846  0.6422920174864777 10.8353848893587461   F   F   F
 10.0412237474326655  5.2906616726497395 14.4983870481855153   T   T   T
  8.3679691075482392  2.6637045915440174 13.6865505739934985   T   T   T
 10.0412397674310956  3.2944539711305953 14.5695081085034346   T   T   T
  8.3674401902338573  0.6375157097460340 13.6778119157221738   T   T   T
  8.3674099101508741  5.0996635089010640 16.9938427445077984   T   T   T
 10.0412964386465990  2.6133782272397799 16.5631043162941509   T   T   T
  8.3672698794946267  3.2507790519011168 17.3121337119070802   T   T   T
 10.0412505052372651  0.5987497027366064 16.4595471217018847   T   T   T
 13.3882312748988763  5.3503169460745283  8.9451241821253618   F   F   F
 11.7146941459090215  2.6726542696091213  8.0000001838787966   F   F   F
 13.3882318235610942  3.3199547705521724  8.9451248436730744   F   F   F
 11.7146932190788640  0.6422920909319076  8.0000000000000000   F   F   F
 11.7146967824986987  5.3503168726290991 11.7805090714841079   F   F   F
 13.3882380226088422  2.6726541961636912 10.8353850732375427   F   F   F
 11.7146973311609131  3.3199546971067431 11.7805097330318205   F   F   F
 13.3882370957786865  0.6422920174864777 10.8353848893587461   F   F   F
 13.3883180109279980  5.2921433222891840 14.4996084988144176   T   T   T
 11.7144932259974439  2.6636719843167920 13.6865291994252498   T   T   T
 13.3882994909452879  3.2953404480922037 14.5683471581940118   T   T   T
 11.7150182559960676  0.6374980222836517 13.6778218306254864   T   T   T
 11.7151227958677300  5.0997206514645486 16.9938274794003306   T   T   T
 13.3883210740746943  2.6145485762338652 16.5607160814372243   T   T   T
 11.7152848822350482  3.2508251625300337 17.3121439660717016   T   T   T
 13.3883405214260023  0.5994208120067327 16.4599656963432537   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_5x2/Rh E_tot= -207.2243487 eV
 D3-zero damping= -10.0205066 eV, D3-BJ damping= -12.084476 eV
Rh
 1.0000000000000000
    13.3883134764000005    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3553253905600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.8120708806377266
  30
Cartesian
  0.0000015735558735 -0.0000003022047019  8.0640486837098688
  1.3388365999338525  1.3388306189696968  9.9060629046204305
 -0.0000006133520801 -0.0000004808802393 11.7480664731683966
  0.0000014783003029  2.6776629713824702  8.0640472578931206
  1.3388380980973364  4.0164947473868695  9.9060624455238830
 -0.0000004441400886  2.6776629659755260 11.7480620451700410
  2.6776556816116628  0.0000008301139574  8.0640204873726251
  4.0164896920179629  1.3388314655612112  9.9060208912888115
  2.6776699884050297  0.0000005789741324 11.7480554451586201
  2.6776560261092262  2.6776618334289175  8.0640218336108571
  4.0164867595971447  4.0164939106070179  9.9060206524589738
```

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  2.6776688067886116  2.6776620263170807 11.7480563113243281
  5.3553198957408021 -0.0000006995024032  8.0639915081945990
  6.6941533927477535  1.3388312278018311  9.9059822719087265
  5.3553299522079492 -0.0000004121867643 11.7480097739750917
  5.3553197199268388  2.6776633630452773  8.0639908809743908
  6.6941517453553585  4.0164941941103969  9.9059831596005026
  5.3553302032805474  2.6776631194419283 11.7480099823314816
  8.0329893303613868 -0.0000007823388783  8.0639784674662955
  9.3718184654924119  1.3388308214816200  9.9059950591545043
  8.0329848130547070 -0.0000000985100545 11.7479902803763245
  8.0329892139270171  2.6776633538559897  8.0639777962518497
  9.3718199601958823  4.0164946270763870  9.9059952390782708
  8.0329852384551277  2.6776631353163185 11.7479886656896628
 10.7106603544526493  0.0000000805774381  8.0640103283395721
 12.0494853876834718  1.3388305020567142  9.9060499080785007
 10.7106431252375742  0.0000000802140194 11.7480232522523362
 10.7106599300942253  2.6776626464396869  8.0640130831509236
 12.0494871939817951  4.0164948466222068  9.9060497552184739
 10.7106436033207544  2.6776625978132556 11.7480232471187733

Interface: ZnO(10-10)/fcc(100)_5x2/Os E_tot= -606.01394979 eV
 D3-zero damping= -23.7705427 eV, D3-BJ damping= -26.4419467 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Os
 1.0000000000000000
    13.5420714154000024    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4168285661600013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.1824709295180504
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2  30
Selective dynamics
Cartesian
  3.3854347083066387  5.4117626022488725  8.9451241821253618   F   F   F
  1.6926778605488420  2.7033483381995405  8.0000001838787966   F   F   F
  3.3854352632699607  3.3580827546327026  8.9451248436730744   F   F   F
  1.6926769230745131  0.6496684873922814  8.0000000000000000   F   F   F
  1.6926805274184020  5.4117625279599588 11.7805090714841079   F   F   F
  3.3854415335106061  2.7033482639106272 10.8353850732375427   F   F   F
  1.6926810823817240  3.3580826803437898 11.7805097330318205   F   F   F
  3.3854405960362777  0.6496684131033682 10.8353848893587461   F   F   F
  3.3629697069206661  5.3761387260111428 14.4703736995892864   T   T   T
  1.6632525898839625  2.6962090015530085 13.6908615824840254   T   T   T
  3.3858014630366235  3.3641868934143728 14.5402012156985396   T   T   T
  1.6755568750881016  0.6689702995270081 13.6545116797042070   T   T   T
  1.6433090738539260  5.5878670149001799 17.3146086221295938   T   T   T
  3.4454345601581959  2.6960748656941802 16.4304100717857082   T   T   T
  1.8688450801153400  3.5250569929256423 17.3631076375534690   T   T   T
  3.3609577938526560  0.7086290662661660 16.3223207385321913   T   T   T
  6.7709525621566389  5.4117626022488725  8.9451241821253618   F   F   F
  5.0781957143988432  2.7033483381995405  8.0000001838787966   F   F   F
  6.7709531171199622  3.3580827546327026  8.9451248436730744   F   F   F
  5.0781947769245139  0.6496684873922814  8.0000000000000000   F   F   F
  5.0781983812684022  5.4117625279599588 11.7805090714841079   F   F   F
  6.7709593873606071  2.7033482639106272 10.8353850732375427   F   F   F
  5.0781989362317246  3.3580826803437898 11.7805097330318205   F   F   F
  6.7709584498862778  0.6496684131033682 10.8353848893587461   F   F   F
  6.7708488965557780  5.3563020510274200 14.4510519199390508   T   T   T
  5.0698352859742792  2.6690864710470552 13.6467307082021083   T   T   T
  6.7709356042144702  3.3491604554033398 14.5052775950761461   T   T   T
  5.0669695874664535  0.6512598517032905 13.6585323235905669   T   T   T
  5.0512853278159540  5.5037979111030166 17.1912839565503042   T   T   T
  6.7709754914035774  2.6574533050167739 16.3860997838129911   T   T   T
  5.1536389870143413  3.4505794465328363 17.2561700607309270   T   T   T
```

6.7709373961581649	0.6761853601936857	16.3005118639837931	T	T	T
10.1564704160066395	5.4117626022488725	8.9451241821253618	F	F	F
8.4637135682488420	2.7033483381995405	8.0000001838787966	F	F	F
10.1564709709699610	3.3580827546327026	8.9451248436730744	F	F	F
8.4637126307745145	0.6496684873922814	8.0000000000000000	F	F	F
8.4637162351184045	5.4117625279599588	11.7805090714841079	F	F	F
10.1564772412106077	2.7033482639106272	10.8353850732375427	F	F	F
8.4637167900817243	3.3580826803437898	11.7805097330318205	F	F	F
10.1564763037362802	0.6496684131033682	10.8353848893587461	F	F	F
10.1788931500232085	5.3760135661204105	14.4704347765612962	T	T	T
8.4720345050553707	2.6689963025906414	13.6467240057883590	T	T	T
10.1561257274147430	3.3640498709859354	14.5401205845545132	T	T	T
8.4748377912202777	0.6511689738928949	13.6585873432923766	T	T	T
8.4904487414164418	5.5035290228664540	17.1912622085097198	T	T	T
10.0965839250323732	2.6958065759835135	16.4303055697017548	T	T	T
8.3884954938183949	3.4503421593281551	17.2561241307275495	T	T	T
10.1809128731690617	0.7083617368586861	16.3223821999030143	T	T	T
13.5419882698566418	5.4117626022488725	8.9451241821253618	F	F	F
11.8492314220988444	2.7033483381995405	8.0000001838787966	F	F	F
13.5419888248199651	3.3580827546327026	8.9451248436730744	F	F	F
11.8492304846245151	0.6496684873922814	8.0000000000000000	F	F	F
11.8492340889684069	5.4117625279599588	11.7805090714841079	F	F	F
13.5419950950606101	2.7033482639106272	10.8353850732375427	F	F	F
11.8492346439317267	3.3580826803437898	11.7805097330318205	F	F	F
13.5419941575862826	0.6496684131033682	10.8353848893587461	F	F	F
13.5419719655631070	5.3780703776047245	14.4957264124918268	T	T	T
11.8786962180174260	2.6961932642414230	13.6908010210519304	T	T	T
13.5419953550106005	3.3658891707942784	14.6846212327677588	T	T	T
11.8662785666990889	0.6689361465416599	13.6545138912323072	T	T	T
11.8986417064584682	5.5876540138909894	17.3146409752977597	T	T	T
13.5419355268135888	2.7562573668225867	16.6552778822507186	T	T	T
11.6730997205328961	3.5248315282488405	17.3628868359939013	T	T	T
13.5419563081170349	0.7538554276667973	16.3273667972172909	T	T	T
0.0002127490149045	0.9733847323572105	19.4439184794709661	T	T	T
1.3514878382710303	2.3195425410727921	21.2916168569278170	T	T	T
0.0000978435836501	0.9769604320742448	23.1427733723213542	T	T	T
0.0002351983214870	3.6757903681361048	19.4798098620204243	T	T	T
1.3664785420929619	5.0140496685159208	21.3014476605554286	T	T	T
0.0002424818578142	3.6977989498583974	23.1592978660053461	T	T	T
2.7243712909410394	0.9982665443859240	19.4930057385658877	T	T	T
4.0507816735602358	2.4159115108803562	21.2779372981527573	T	T	T
2.7531651991816601	0.9949531261272704	23.1306802947002303	T	T	T
2.6313726738173928	3.6760935022747185	19.3713410947893365	T	T	T
4.0549974046377484	5.0021504711853160	21.2356185537550672	T	T	T
2.7063430198614111	3.7126916841382274	23.1708581306609922	T	T	T
5.4171896769828942	1.0267403877880406	19.5221034055026159	T	T	T
6.7712884354396126	2.4575736334721703	21.2805802400941033	T	T	T
5.4552925823029872	1.0162167542306575	23.1179574109981374	T	T	T
5.3775516573645703	3.6852749034613566	19.3345128152132979	T	T	T
6.7713513923752870	5.0179548677228620	21.2115603439531171	T	T	T
5.4136290098322757	3.7487043738187391	23.1530221187330660	T	T	T
8.1253938641407970	1.0267487542434084	19.5220563581827449	T	T	T
9.4917435542789104	2.4159056455421601	21.2780045092985759	T	T	T
8.0872363480241276	1.0161860729588301	23.1179716657277723	T	T	T
8.1648909563938528	3.6851875001125385	19.3345255750394678	T	T	T
9.4876787208958895	5.0021804676038117	21.2354331889929568	T	T	T
8.1290653110464088	3.7487524508809491	23.1529721151815622	T	T	T
10.8183484405330752	0.9983698270419280	19.4930861481456894	T	T	T
12.1910232699023684	2.3196653183380813	21.2916859029284922	T	T	T
10.7893334495511528	0.9949590392968025	23.1306733428594917	T	T	T
10.9111099865971468	3.6760657705481341	19.3713101603391351	T	T	T
12.1761546421319746	5.0139983300332958	21.3013816976201831	T	T	T
10.8361890117713209	3.7127646427861203	23.1708709768837373	T	T	T

```
Oxide reference: ZnO(10-10)/fcc(100)_5x2/Os E_tot= -286.71644354 eV
 D3-zero damping= -10.2152436 eV, D3-BJ damping= -10.9610225 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O
 1.0000000000000000
    13.5420714154000024    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4168285661600013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.9371186129033156
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.3854347083066387  5.4117626022488725  8.9451241821253618   F   F   F
  1.6926778605488420  2.7033483381995405  8.0000001838787966   F   F   F
  3.3854352632699607  3.3580827546327026  8.9451248436730744   F   F   F
  1.6926769230745131  0.6496684873922814  8.0000000000000000   F   F   F
  1.6926805274184020  5.4117625279599588 11.7805090714841079   F   F   F
  3.3854415335106061  2.7033482639106272 10.8353850732375427   F   F   F
  1.6926810823817240  3.3580826803437898 11.7805097330318205   F   F   F
  3.3854405960362777  0.6496684131033682 10.8353848893587461   F   F   F
  3.3851995544876621  5.3415866523004896 14.4642168617512130   T   T   T
  1.6914789027198407  2.6855197381200693 13.6786640392523573   T   T   T
  3.3852920923920622  3.3364450173054858 14.5244943373263524   T   T   T
  1.6913532878162711  0.6460742968667484 13.6768380007388828   T   T   T
  1.6933435028195400  5.1569511380810260 16.9218428354941466   T   T   T
  3.3851953351466322  2.6360657197433692 16.5146836314959380   T   T   T
  1.6926428109800569  3.2979842341262011 17.2155903486063053   T   T   T
  3.3852812301615973  0.6057380559957590 16.4299876337196658   T   T   T
  6.7709525621566389  5.4117626022488725  8.9451241821253618   F   F   F
  5.0781957143988432  2.7033483381995405  8.0000001838787966   F   F   F
  6.7709531171199622  3.3580827546327026  8.9451248436730744   F   F   F
  5.0781947769245139  0.6496684873922814  8.0000000000000000   F   F   F
  5.0781983812684022  5.4117625279599588 11.7805090714841079   F   F   F
  6.7709593873606071  2.7033482639106272 10.8353850732375427   F   F   F
  5.0781989362317246  3.3580826803437898 11.7805097330318205   F   F   F
  6.7709584498862778  0.6496684131033682 10.8353848893587461   F   F   F
  6.7707843686171865  5.3425840601717001 14.4690099951125646   T   T   T
  5.0791384114202369  2.6854868521169291 13.6786717460031380   T   T   T
  6.7708042069368339  3.3376365503302803 14.5264613706550385   T   T   T
  5.0790790356540763  0.6460650988407644 13.6768328578382548   T   T   T
  5.0772207835587011  5.1570067815205487 16.9218143878449894   T   T   T
  6.7707250772345811  2.6372084759241088 16.5163374852679787   T   T   T
  5.0777572577044339  3.2980045901776798 17.2155817083006539   T   T   T
  6.7708274080788531  0.6056611589904368 16.4333159443637022   T   T   T
 10.1564704160066395  5.4117626022488725  8.9451241821253618   F   F   F
  8.4637135682488420  2.7033483381995405  8.0000001838787966   F   F   F
 10.1564709709699610  3.3580827546327026  8.9451248436730744   F   F   F
  8.4637126307745145  0.6496684873922814  8.0000000000000000   F   F   F
  8.4637162351184045  5.4117625279599588 11.7805090714841079   F   F   F
 10.1564772412106077  2.7033482639106272 10.8353850732375427   F   F   F
  8.4637167900817243  3.3580826803437898 11.7805097330318205   F   F   F
 10.1564763037362802  0.6496684131033682 10.8353848893587461   F   F   F
 10.1562336259658874  5.3415863045067988 14.4642138709207160   T   T   T
  8.4625133483544523  2.6855195615342162 13.6786639966965637   T   T   T
 10.1563287565687546  3.3364451442737919 14.5244939670741573   T   T   T
  8.4623898699888453  0.6460743213554437 13.6768373820980376   T   T   T
  8.4643981963160417  5.1569586163413872 16.9218873675365273   T   T   T
 10.1562308056932569  2.6360671244845539 16.5146805474492773   T   T   T
  8.4636795347141636  3.2979831479971740 17.2155914225310767   T   T   T
 10.1563225960126520  0.6057414275247942 16.4299878635926007   T   T   T
 13.5419882698566418  5.4117626022488725  8.9451241821253618   F   F   F
 11.8492314220988444  2.7033483381995405  8.0000001838787966   F   F   F
```

```
 13.5419888248199651  3.3580827546327026  8.9451248436730744   F   F   F
 11.8492304846245151  0.6496684873922814  8.0000000000000000   F   F   F
 11.8492340889684069  5.4117625279599588 11.7805090714841079   F   F   F
 13.5419950950606101  2.7033482639106272 10.8353850732375427   F   F   F
 11.8492346439317267  3.3580826803437898 11.7805097330318205   F   F   F
 13.5419941575862826  0.6496684131033682 10.8353848893587461   F   F   F
 13.5418192305152729  5.3425838572318165 14.4690061170437243   T   T   T
 11.8501746574750690  2.6854870606812349 13.6786712123326986   T   T   T
 13.5418401197775164  3.3376370195568672 14.5264626131500165   T   T   T
 11.8501157256788279  0.6460651662252186 13.6768335693667087   T   T   T
 11.8482559818047619  5.1570054751810348 16.9218141261076092   T   T   T
 13.5417617924834151  2.6372097232168072 16.5163395685368002   T   T   T
 11.8487926764312164  3.2980050201957050 17.2155815707981219   T   T   T
 13.5418513536702072  0.6056671131921030 16.4333118815308019   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_5x2/Os E_tot= -309.06365752 eV
 D3-zero damping= -9.6363574 eV, D3-BJ damping= -11.550738 eV
Os
 1.0000000000000000
    13.5420714154000024    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4168285661600013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.8120708806377266
  30
Cartesian
  0.0000002350087274 -0.0000004842514394  8.0540640369513437
  1.3542090322037019  1.3542065777626480  9.9060365543716991
 -0.0000005870396666 -0.0000007358161320 11.7580432501712338
  0.0000004159023018  2.7084147119941608  8.0540631064948460
  1.3542115118862097  4.0626219657436495  9.9060359139013521
  0.0000003570567539  2.7084149794047954 11.7580406091492886
  2.7084087970053394  0.0000014765449207  8.0540440714962216
  4.0626204984313441  1.3542072323979342  9.9060137787990303
  2.7084192043976265  0.0000012940086695 11.7580328367831743
  2.7084103110442386  2.7084127887191851  8.0540447563652915
  4.0626167341847630  4.0626213387375705  9.9060133112085111
  2.7084164304666820  2.7084129830078756 11.7580331352578984
  5.4168269146954549 -0.0000020188048844  8.0540185508516355
  6.7710349750143219  1.3542072215479755  9.9059925017981669
  5.4168307498859019 -0.0000018542359016 11.7579975720273762
  5.4168258139592291  2.7084163268558501  8.0540181288912471
  6.7710337922061390  4.0626212880892121  9.9059938739468585
  5.4168326920409413  2.7084160634207430 11.7579974860939185
  8.1252416539624761 -0.0000035527521526  8.0540068535618055
  9.4794490744686399  1.3542066378849225  9.9059979111126779
  8.1252403548024645 -0.0000029796489178 11.7579843441981229
  8.1252418489456844  2.7084176941706581  8.0540057463845685
  9.4794508040955439  4.0626220445753658  9.9059982658546986
  8.1252397394403459  2.7084175565514834 11.7579837444586612
 10.8336654022353116 -0.0000018259090996  8.0540318083078422
 12.1878649635372920  1.3542064162775234  9.9060293366075118
 10.8336530239963622 -0.0000017962110022 11.7580120708332387
 10.8336637638421216  2.7084160990315400  8.0540344703199285
 12.1878658052676148  4.0626222085416765  9.9060291605448647
 10.8336540843275628  2.7084161480120579 11.7580110071446367

Interface: ZnO(10-10)/fcc(100)_5x2/Ru E_tot= -554.79739196 eV
 D3-zero damping= -25.0669422 eV, D3-BJ damping= -26.6559917 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Ru
 1.0000000000000000
    13.3309737097000021    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3323894838800010    0.0000000000000000
     0.0000000000000000    0.0000000000000000   31.1824709295180504
```

```
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2  30
Selective dynamics
Cartesian
  3.3326615779782918  5.3274024896719538  8.9451241821253618   F   F   F
  1.6662919110223386  2.6612077664659672  8.0000001838787966   F   F   F
  3.3326621242906858  3.3057359944282361  8.9451248436730744   F   F   F
  1.6662909881616295  0.6395412680809034  8.0000000000000000   F   F   F
  1.6662945363199688  5.3274024165410783 11.7805090714841079   F   F   F
  3.3326682967890160  2.6612076933350908 10.8353850732375427   F   F   F
  1.6662950826323626  3.3057359212973605 11.7805097330318205   F   F   F
  3.3326673739283073  0.6395411949500270 10.8353848893587461   F   F   F
  3.3140136434229799  5.3047110345183173 14.5257147984960540   T   T   T
  1.6522392282589540  2.6660815345745026 13.6908225385684439   T   T   T
  3.3274388773823191  3.3036890281467852 14.6122706624914418   T   T   T
  1.6566845925195404  0.6556481193370062 13.6574984081474771   T   T   T
  1.6105944481311405  5.5003998741136240 17.3985909671712307   T   T   T
  3.3542644146665035  2.6708505365485351 16.5246570461166584   T   T   T
  1.7274801482183726  3.4446112911737230 17.4385871674347577   T   T   T
  3.2928092272664613  0.6886565168261179 16.3862463281349697   T   T   T
  6.6654050054032918  5.3274024896719538  8.9451241821253618   F   F   F
  4.9990353384473396  2.6612077664659672  8.0000001838787966   F   F   F
  6.6654055517156863  3.3057359944282361  8.9451248436730744   F   F   F
  4.9990344155866300  0.6395412680809034  8.0000000000000000   F   F   F
  4.9990379637449687  5.3274024165410783 11.7805090714841079   F   F   F
  6.6654117242140165  2.6612076933350908 10.8353850732375427   F   F   F
  4.9990385100573622  3.3057359212973605 11.7805097330318205   F   F   F
  6.6654108013533069  0.6395411949500270 10.8353848893587461   F   F   F
  6.6640154387643555  5.2826495059724587 14.5078386466150118   T   T   T
  4.9866421885404248  2.6465454722428041 13.6709939195928332   T   T   T
  6.6640449937339339  3.2852670812909044 14.5721064340334632   T   T   T
  4.9878959685285125  0.6369003886569188 13.6663396628156946   T   T   T
  4.9583452666507126  5.4168917315995495 17.2851932146332032   T   T   T
  6.6639095218434639  2.6214900158232224 16.4761939462273084   T   T   T
  5.0460722625908367  3.3793717759880848 17.3345191612748017   T   T   T
  6.6636392784211305  0.6471395701758570 16.3736054584157706   T   T   T
  9.9981484328282928  5.3274024896719538  8.9451241821253618   F   F   F
  8.3317787658723397  2.6612077664659672  8.0000001838787966   F   F   F
  9.9981489791406855  3.3057359944282361  8.9451248436730744   F   F   F
  8.3317778430116292  0.6395412680809034  8.0000000000000000   F   F   F
  8.3317813911699705  5.3274024165410783 11.7805090714841079   F   F   F
  9.9981551516390166  2.6612076933350908 10.8353850732375427   F   F   F
  8.3317819374823632  3.3057359212973605 11.7805097330318205   F   F   F
  9.9981542287783096  0.6395411949500270 10.8353848893587461   F   F   F
 10.0144115464265440  5.3042313556364995 14.5256721870031367   T   T   T
  8.3410180763780488  2.6459552509595468 13.6703920607506753   T   T   T
 10.0006286088277214  3.3032490054531811 14.6103452651899293   T   T   T
  8.3401330626369514  0.6365737820034711 13.6664100662679608   T   T   T
  8.3686025042417835  5.4159435881181128 17.2847950080205592   T   T   T
  9.9723301595737794  2.6691279717094050 16.5222200564915909   T   T   T
  8.2827178505518422  3.3782861047802455 17.3340915164930855   T   T   T
 10.0349130439606142  0.6870524356659086 16.3865787437811647   T   T   T
 13.3308918602532938  5.3274024896719538  8.9451241821253618   F   F   F
 11.6645221932973406  2.6612077664659672  8.0000001838787966   F   F   F
 13.3308924065656882  3.3057359944282361  8.9451248436730744   F   F   F
 11.6645212704366301  0.6395412680809034  8.0000000000000000   F   F   F
 11.6645248185949715  5.3274024165410783 11.7805090714841079   F   F   F
 13.3308985790640175  2.6612076933350908 10.8353850732375427   F   F   F
 11.6645253649073641  3.3057359212973605 11.7805097330318205   F   F   F
 13.3308976562033106  0.6395411949500270 10.8353848893587461   F   F   F
 13.3298781818355447  5.3170475404749373 14.5282930987684740   T   T   T
 11.6767175582238512  2.6660470111889829 13.6910094139184455   T   T   T
 13.3300037480116931  3.3170123964367701 14.6678489532899707   T   T   T
```

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 11.6719083788304996  0.6555569943432679 13.6576430805579001   T   T   T
 11.7190214163817856  5.4980776923009200 17.3968621152829250   T   T   T
 13.3283580522015050  2.7217700129383475 16.6041070631430188   T   T   T
 11.5971916235104189  3.4426876165930782 17.4348356586520445   T   T   T
 13.3298951180606480  0.7331123684909212 16.3730178630421861   T   T   T
  0.0045049446635074  1.0844965535681947 19.4743620524125056   T   T   T
  1.3356385118125720  2.3841768586780407 21.2833840081151529   T   T   T
  0.0059098571720500  1.0766891339815838 23.0926243648095486   T   T   T
  0.0061711092294831  3.7413827096107184 19.4589009669959303   T   T   T
  1.3366544000028979  5.0594396970402524 21.2341582422141926   T   T   T
  0.0029217290899976  3.7766166570229789 23.1102845552505336   T   T   T
  2.7122870874665890  1.1317188182010418 19.5052922539304490   T   T   T
  3.9962217334310339  2.5090615272522285 21.3216585149937821   T   T   T
  2.7317228166768142  1.1062361692789511 23.1076650925293485   T   T   T
  2.6282323069459310  3.7436281839212238 19.4001014870671327   T   T   T
  3.9955075289730693  5.0672853105857998 21.1935531197400948   T   T   T
  2.6471938729906408  3.8267608815617136 23.1161797164213745   T   T   T
  5.3583759139547773  1.1833799256621191 19.5316873761086534   T   T   T
  6.6691844947977996  2.5648790700242987 21.3584386557497439   T   T   T
  5.3820536701159352  1.1609554366178272 23.1329638944412430   T   T   T
  5.3124498523418398  3.7486581151237997 19.3856788297406020   T   T   T
  6.6697275062973285  5.0945379834303219 21.1772619777128526   T   T   T
  5.3181992436277801  3.9115975130307059 23.1231471798363302   T   T   T
  7.9822950305051741  1.1833058931069709 19.5323352603032951   T   T   T
  9.3444877022000892  2.5051905013737104 21.3227552698475975   T   T   T
  7.9527822551915603  1.1598817533979702 23.1340370800893638   T   T   T
  8.0264601161971072  3.7479742816853019 19.3856993654811625   T   T   T
  9.3446808632240828  5.0654190175003420 21.1936658712018762   T   T   T
  8.0224783086404603  3.9111207107972765 23.1231285850040820   T   T   T
 10.6277137133515716  1.1303549748886874 19.5055827780452233   T   T   T
 12.0037787061047041  2.3848111808452517 21.2826066940868301   T   T   T
 10.6063725507779676  1.1060981924614692 23.1089915702436279   T   T   T
 10.7115652061168731  3.7427380057852462 19.3993141158360984   T   T   T
 12.0057374746916992  5.0560821277047063 21.2318953974415052   T   T   T
 10.6917188631134756  3.8282789502125683 23.1161950301299761   T   T   T

Oxide reference: ZnO(10-10)/fcc(100)_5x2/Ru E_tot= -287.55304032 eV
 D3-zero damping= -10.3365277 eV, D3-BJ damping= -11.2268104 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O
 1.0000000000000000
    13.3309737097000021    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3323894838800010    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.9371186129033156
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.3326615779782918  5.3274024896719538  8.9451241821253618   F   F   F
  1.6662919110223386  2.6612077664659672  8.0000001838787966   F   F   F
  3.3326621242906858  3.3057359944282361  8.9451248436730744   F   F   F
  1.6662909881616295  0.6395412680809034  8.0000000000000000   F   F   F
  1.6662945363199688  5.3274024165410783 11.7805090714841079   F   F   F
  3.3326682967890160  2.6612076933350908 10.8353850732375427   F   F   F
  1.6662950826323626  3.3057359212973605 11.7805097330318205   F   F   F
  3.3326673739283073  0.6395411949500270 10.8353848893587461   F   F   F
  3.3327796436007775  5.2740277184849633 14.5138915076194550   T   T   T
  1.6667857787401965  2.6552533500424840 13.6883420215123266   T   T   T
  3.3327775463049059  3.2792853377574538 14.5849016488575316   T   T   T
  1.6664362069258751  0.6338984617357163 13.6774988342559549   T   T   T
  1.6650797449815840  5.0767340646685106 17.0231805478173008   T   T   T
  3.3328178510127557  2.6039572085279956 16.5763173362618303   T   T   T
  1.6661418886836377  3.2308185372672451 17.3465138779889863   T   T   T
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  3.3327673000729461  0.5940717184649257 16.4721231061856841   T   T   T
  6.6654050054032918  5.3274024896719538  8.9451241821253618   F   F   F
  4.9990353384473396  2.6612077664659672  8.0000001838787966   F   F   F
  6.6654055517156863  3.3057359944282361  8.9451248436730744   F   F   F
  4.9990344155866300  0.6395412680809034  8.0000000000000000   F   F   F
  4.9990379637449687  5.3274024165410783 11.7805090714841079   F   F   F
  6.6654117242140165  2.6612076933350908 10.8353850732375427   F   F   F
  4.9990385100573622  3.3057359212973605 11.7805097330318205   F   F   F
  6.6654108013533069  0.6395411949500270 10.8353848893587461   F   F   F
  6.6655152251166569  5.2745459439379241 14.5116819401806474   T   T   T
  4.9987556885276483  2.6552531717614309 13.6882964625397889   T   T   T
  6.6655101239449257  3.2799846418990755 14.5836313124962373   T   T   T
  4.9990984275372723  0.6339068387814883 13.6774917513854373   T   T   T
  5.0005006218599704  5.0767952254654540 17.0232349232551172   T   T   T
  6.6655136935830113  2.6057416173524865 16.5749009339978706   T   T   T
  4.9994080044381315  3.2308911351107588 17.3466083122849604   T   T   T
  6.6655211485402353  0.5957008719489802 16.4707240181762096   T   T   T
  9.9981484328282928  5.3274024896719538  8.9451241821253618   F   F   F
  8.3317787658723397  2.6612077664659672  8.0000001838787966   F   F   F
  9.9981489791406855  3.3057359944282361  8.9451248436730744   F   F   F
  8.3317778430116292  0.6395412680809034  8.0000000000000000   F   F   F
  8.3317813911699705  5.3274024165410783 11.7805090714841079   F   F   F
  9.9981551516390166  2.6612076933350908 10.8353850732375427   F   F   F
  8.3317819374823632  3.3057359212973605 11.7805097330318205   F   F   F
  9.9981542287783096  0.6395411949500270 10.8353848893587461   F   F   F
  9.9982659410194241  5.2740225653035129 14.5139016166341577   T   T   T
  8.3322906912969632  2.6552456325730387 13.6883278932844750   T   T   T
  9.9982721177189759  3.2792799870986387 14.5849111868577559   T   T   T
  8.3319328385257840  0.6338944900890116 13.6774976266487727   T   T   T
  8.3305702176751488  5.0767197195418881 17.0231856307721579   T   T   T
  9.9982932533727826  2.6039408117160030 16.5763181732995690   T   T   T
  8.3316333857854179  3.2308096209413542 17.3465354761232255   T   T   T
  9.9982477792771416  0.5940660768554842 16.4721252779391207   T   T   T
 13.3308918602532938  5.3274024896719538  8.9451241821253618   F   F   F
 11.6645221932973406  2.6612077664659672  8.0000001838787966   F   F   F
 13.3308924065656882  3.3057359944282361  8.9451248436730744   F   F   F
 11.6645212704366301  0.6395412680809034  8.0000000000000000   F   F   F
 11.6645248185949715  5.3274024165410783 11.7805090714841079   F   F   F
 13.3308985790640175  2.6612076933350908 10.8353850732375427   F   F   F
 11.6645253649073641  3.3057359212973605 11.7805097330318205   F   F   F
 13.3308976562033106  0.6395411949500270 10.8353848893587461   F   F   F
 13.3309995244016690  5.2745496328868988 14.5116916752610603   T   T   T
 11.6642430399856529  2.6552502980301926 13.6882994978396546   T   T   T
 13.3309820338110612  3.2799868555095300 14.5836638083513979   T   T   T
 11.6645865071941195  0.6339040350721294 13.6774942154244510   T   T   T
 11.6659871511773225  5.0767982518467401 17.0232447057516154   T   T   T
 13.3309760339227985  2.6057556829587893 16.5748669279866476   T   T   T
 11.6648607925530658  3.2308981156578915 17.3466719708216175   T   T   T
 13.3309998720379816  0.5957185149872192 16.4707347337566254   T   T   T

Metal reference: ZnO(10-10)/fcc(100)_5x2/Ru E_tot= -256.21869134 eV
 D3-zero damping= -9.4633972 eV, D3-BJ damping= -11.5432159 eV
Ru
 1.0000000000000000
    13.3309737097000021    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3323894838800010    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.8120708806377266
  30
Cartesian
  0.0000679631520086 -0.0000021172437073  8.0741178034811298
  1.3333746736619085  1.3330958217900348  9.9060318054232379
  0.0000456172418877 -0.0000019831956940 11.7379249604961586
  0.0000579966949960  2.6661944882328741  8.0741583223161104
```

```
  1.3333798328409303  3.9992914228065635  9.9060303022676344
  0.0000472605204720  2.6661937694303814 11.7379201708327709
  2.6661074952290669  0.0000006341276498  8.0738644105895521
  3.9994180125057097  1.3330955585675592  9.9059883534195023
  2.6661341900308053  0.0000001183004899 11.7381730069100758
  2.6661043630097829  2.6661919430689998  8.0738648594305147
  3.9994131186643904  3.9992909002082317  9.9059869208261357
  2.6661324792819778  2.6661921734274880 11.7381744243958330
  5.3324120276213236 -0.0000033505372450  8.0737247676879207
  6.6653877401353796  1.3330933620923724  9.9059688968504034
  5.3324165281226792 -0.0000027131747306 11.7382405675174279
  5.3324082651199776  2.6661947830458748  8.0737258039192135
  6.6653877169138500  3.9992954918721804  9.9059684521099189
  5.3324213667075950  2.6661958816144957 11.7382382641709526
  7.9985331767782819  0.0000230020942361  8.0737536220521786
  9.3314812141287504  1.3330928891493881  9.9059865813320673
  7.9985024285229969 -0.0000040554309435 11.7383509414579397
  7.9985336232752946  2.6662012226421172  8.0738284490382366
  9.3314820943301253  3.9992962833270673  9.9059847146644415
  7.9985006498616711  2.6661983744152611 11.7383528372768069
 10.6647909430244638 -0.0000037103222885  8.0741327006230694
 11.9979349206478147  1.3330949724868937  9.9060209337379792
 10.6647292549064048 -0.0000025689463772 11.7379705643612802
 10.6647919656454544  2.6661951493182774  8.0741375887538105
 11.9979345532013664  3.9992912008660637  9.9060209552566114
 10.6647269101868627  2.6661958349110342 11.7379663675154156

Interface: ZnO(10-10)/fcc(111)_2sqrt3x2/Au E_tot= -300.07307491 eV
 D3-zero damping= -21.9383635 eV, D3-BJ damping= -21.1082234 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Au
 1.0000000000000000
    10.0415704821224576    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7975034209400009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.1021996581789182
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2  24
Selective dynamics
Cartesian
  3.3471079564608490  5.7920814396558580  8.9451241821253618   F   F   F
  1.6735149317359077  2.8933297495539323  8.0000001838787966   F   F   F
  3.3471085051413918  3.5940765006679847  8.9451248436730744   F   F   F
  1.6735140048747938  0.6953248071507115  8.0000000000000000   F   F   F
  1.6735175684136441  5.7920813601461925 11.7805090714841079   F   F   F
  3.3471147043961880  2.8933296700442663 10.8353850732375427   F   F   F
  1.6735181170941860  3.5940764211583196 11.7805097330318205   F   F   F
  3.3471137775350748  0.6953247276410457 10.8353848893587461   F   F   F
  3.3311998549895776  5.6951194400050733 14.4528186286525866   T   T   T
  1.6773184408830297  2.8293508201646387 13.6414796558576548   T   T   T
  3.3377752165409542  3.6233195963479732 14.5074813521926416   T   T   T
  1.6646193533942537  0.7179538793171008 13.6537514455017881   T   T   T
  1.6751898989749228  5.7369173536438911 17.0628812996066763   T   T   T
  3.3166950150592993  2.8939555599922051 16.4501563698555771   T   T   T
  1.6007433801595203  3.7387544760371707 17.0343168983757103   T   T   T
  3.3286697832636238  0.7955109587036657 16.3182083542969103   T   T   T
  6.6942981171683344  5.7920814396558580  8.9451241821253618   F   F   F
  5.0207050924433938  2.8933297495539323  8.0000001838787966   F   F   F
  6.6942986658488772  3.5940765006679847  8.9451248436730744   F   F   F
  5.0207041655822797  0.6953248071507115  8.0000000000000000   F   F   F
  5.0207077291211295  5.7920813601461925 11.7805090714841079   F   F   F
  6.6943048651036747  2.8933296700442663 10.8353850732375427   F   F   F
  5.0207082778016714  3.5940764211583196 11.7805097330318205   F   F   F
  6.6943039382425606  0.6953247276410457 10.8353848893587461   F   F   F
  6.6841624484629243  5.6693371528871781 14.4349895746868846   T   T   T
```

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  4.9949082819561115  2.8234526614195183 13.6381341854276066   T   T   T
  6.6839502961510604  3.6062585454862273 14.4448630701912908   T   T   T
  5.0084656355128701  0.7148667254869363 13.6554915364984630   T   T   T
  4.9948842824207169  5.7494158603440457 17.0252162442823618   T   T   T
  6.6787229046490078  2.7967913622613754 16.3243607937856439   T   T   T
  5.0496745877254519  3.7421538424617462 17.0261753558886149   T   T   T
  6.6992587024208046  0.7319537155126470 16.3092390290698077   T   T   T
 10.0414882778758212  5.7920814396558580  8.9451241821253618   F   F   F
  8.3678952531508788  2.8933297495539323  8.0000001838787966   F   F   F
 10.0414888265563604  3.5940765006679847  8.9451248436730744   F   F   F
  8.3678943262897647  0.6953248071507115  8.0000000000000000   F   F   F
  8.3678978898286172  5.7920813601461925 11.7805090714841079   F   F   F
 10.0414950258111606  2.8933296700442663 10.8353850732375427   F   F   F
  8.3678984385091564  3.5940764211583196 11.7805097330318205   F   F   F
 10.0414940989500465  0.6953247276410457 10.8353848893587461   F   F   F
 -0.0046805015763665  5.6702981563642378 14.4412346111551813   T   T   T
  8.3599940727931159  2.8097091566380739 13.6239967153554176   T   T   T
 10.0299585606562776  3.6062315320198959 14.4513389202282418   T   T   T
  8.3592995034918918  0.7072615108032332 13.6541257840436465   T   T   T
  8.3582974112273352  5.6371252761556301 17.0439223120185126   T   T   T
 10.0231740654135919  2.7956895001043143 16.3443086719462087   T   T   T
  8.3453435484062926  3.6261770615120179 17.0298012047368488   T   T   T
 10.0148055030786107  0.7293583833591162 16.3125368718242640   T   T   T
  0.6350989629041031  0.8905379261044333 19.3581390574724423   T   T   T
  1.7109304059149362  2.6986464288640262 21.8550831706292534   T   T   T
  4.2066813953939448  1.2446268226415151 21.9021554086316321   T   T   T
  2.5597133838872961  1.2817213252534123 24.3295049917147068   T   T   T
  3.1420528008086079  2.2121914717447129 19.3727393600363023   T   T   T
  5.0923388163968477  2.7370927454714407 24.3029240838518490   T   T   T
  0.7072632012411921  3.7747236310192593 19.3709239060791418   T   T   T
  1.6822538764074120  5.6079911634003006 21.8810070803313650   T   T   T
  4.2199118932953326  4.1289722893658949 21.8512085154439184   T   T   T
  2.5754396050188348  4.1822860729984761 24.3125055903588674   T   T   T
  3.1673987600440001  5.2191821895628978 19.4478139302643136   T   T   T
  5.0685633851463221  5.6386568305408353 24.3758482312486500   T   T   T
  5.6889077240626964  0.8496910073396211 19.4184164404677233   T   T   T
  6.7230702763586869  2.7193123211266217 21.6988776118596256   T   T   T
  9.1961967288197553  1.2780852324850582 21.7917392904658662   T   T   T
  7.5835566215400974  1.2969563557052344 24.2776994010433071   T   T   T
  8.2053374300628903  2.4419190407069520 19.1933143414995939   T   T   T
 10.0940222029477678  2.7216630526110070 24.3043516723098030   T   T   T
  5.5856919804541398  3.6974982002223502 19.3058448517699190   T   T   T
  6.6795299329026605  5.5894230110327472 21.9504950342616141   T   T   T
  9.2692188726835756  4.1271283896967663 21.8444367880446109   T   T   T
  7.6017391517789212  4.1706085952219576 24.2979226629564593   T   T   T
  8.1746312802277572  5.3748065560215084 19.5901231026422451   T   T   T
 10.0807792010252673  5.6355602839412811 24.3022697461802721   T   T   T

Oxide reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Au E_tot= -211.99202822 eV
 D3-zero damping= -7.4696597 eV, D3-BJ damping= -7.8397156 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
    10.0415704821224576    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7975034209400009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.3092812387561530
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2
Selective dynamics
Cartesian
  3.3471079564608490  5.7920814396558580  8.9451241821253618   F   F   F
  1.6735149317359077  2.8933297495539323  8.0000001838787966   F   F   F
  3.3471085051413918  3.5940765006679847  8.9451248436730744   F   F   F
  1.6735140048747938  0.6953248071507115  8.0000000000000000   F   F   F
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  1.6735175684136441  5.7920813601461925 11.7805090714841079   F   F   F
  3.3471147043961880  2.8933296700442663 10.8353850732375427   F   F   F
  1.6735181170941860  3.5940764211583196 11.7805097330318205   F   F   F
  3.3471137775350748  0.6953247276410457 10.8353848893587461   F   F   F
  3.3462143014828234  5.6779966580316463 14.4164839494545021   T   T   T
  1.6722288394250531  2.8477123962484998 13.6510724347398025   T   T   T
  3.3457585048196723  3.6182821223615069 14.4622158395790699   T   T   T
  1.6736619349301098  0.7208090932544521 13.6581121274333981   T   T   T
  1.6747538427941091  5.4775540140210586 16.8032449559273829   T   T   T
  3.3471114584757964  2.7863952832217960 16.4299374498666317   T   T   T
  1.6751364303632281  3.5953304866265130 17.0608520705444882   T   T   T
  3.3466655069211519  0.6723763019435801 16.3822785311396615   T   T   T
  6.6942981171683344  5.7920814396558580  8.9451241821253618   F   F   F
  5.0207050924433938  2.8933297495539323  8.0000001838787966   F   F   F
  6.6942986658488772  3.5940765006679847  8.9451248436730744   F   F   F
  5.0207041655822797  0.6953248071507115  8.0000000000000000   F   F   F
  5.0207077291211295  5.7920813601461925 11.7805090714841079   F   F   F
  6.6943048651036747  2.8933296700442663 10.8353850732375427   F   F   F
  5.0207082778016714  3.5940764211583196 11.7805097330318205   F   F   F
  6.6943039382425606  0.6953247276410457 10.8353848893587461   F   F   F
  6.6952800609175362  5.6780080923509972 14.4164719850476750   T   T   T
  5.0207262501549144  2.8481533484588941 13.6515027964357145   T   T   T
  6.6957286869473860  3.6182768519095898 14.4622041759036346   T   T   T
  5.0207471858769974  0.7204631237801074 13.6585269156950080   T   T   T
  5.0207759213394150  5.4777667985531764 16.7984082487631845   T   T   T
  6.6944245992869389  2.7864011296650673 16.4299291933438774   T   T   T
  5.0207782391860922  3.5952904929179854 17.0577909357543192   T   T   T
  6.6948679260434760  0.6723783584339453 16.3822558654272115   T   T   T
 10.0414882778758212  5.7920814396558580  8.9451241821253618   F   F   F
  8.3678952531508788  2.8933297495539323  8.0000001838787966   F   F   F
 10.0414888265563604  3.5940765006679847  8.9451248436730744   F   F   F
  8.3678943262897647  0.6953248071507115  8.0000000000000000   F   F   F
  8.3678978898286172  5.7920813601461925 11.7805090714841079   F   F   F
 10.0414950258111606  2.8933296700442663 10.8353850732375427   F   F   F
  8.3678984385091564  3.5940764211583196 11.7805097330318205   F   F   F
 10.0414940989500465  0.6953247276410457 10.8353848893587461   F   F   F
 -0.0000274887921932  5.6781749721730979 14.4202792011823338   T   T   T
  8.3692877596827593  2.8477109151050315 13.6510853140721817   T   T   T
 10.0415328738032841  3.6182989420753500 14.4652612133057907   T   T   T
  8.3678393980173293  0.7208130193126542 13.6581035150777286   T   T   T
  8.3667904272263733  5.4775745122175508 16.8032386693750198   T   T   T
 10.0415506320630445  2.7874308331551321 16.4387759176293571   T   T   T
  8.3664295463366507  3.5953340619048237 17.0608135794441438   T   T   T
 10.0415574867443453  0.6711850200007352 16.3853592525194465   T   T   T

Metal reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Au E_tot= -82.86484454 eV
 D3-zero damping= -10.3239224 eV, D3-BJ damping= -10.5591296 eV
Au
 1.0000000000000000
    10.0415704821224576    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7975034209400009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.5552264120280803
  24
Cartesian
  0.5591016425220285  0.9874621314813770  7.8282105205054364
  1.4049031642135672  2.4303708123737144 10.2784051959730434
  3.9145774379387110  0.9786017138508500 10.2761413490075633
  2.2504817500210161  0.9864372921440960 12.7279845889698660
  3.0698687504047633  2.4364835944169219  7.8239965697857006
  4.7592721616462992  2.4352232984603241 12.7291633487955114
  0.5590375274146225  3.8859956420994171  7.8282904116886636
  1.4049334182232696  5.3291221816987493 10.2781821666067898
  3.9145939320714480  3.8773688884445412 10.2763128622979796
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  2.2509435903965933  3.8846907926371887 12.7277871280903714
  3.0700527209267676  5.3354478996419967  7.8236435670305697
  4.7590000316058356  5.3335719769795080 12.7290946073345808
  5.5789008327882152  0.9889814490269028  7.8269583145685608
  6.4255502790049706  2.4314860709362005 10.2778379110920870
  8.9355055213959282  0.9796045338373168 10.2784227932739576
  7.2712755360076438  0.9869808643278259 12.7275674665433343
  8.0905546397769967  2.4366646479025986  7.8261569347828175
  9.7803412601711628  2.4360097799214873 12.7303221253105683
  5.5790375736440101  3.8882020737296710  7.8269939680770353
  6.4255122857789635  5.3301594125779133 10.2779657290692796
  8.9356036293510304  3.8779517246532671 10.2784210405868688
  7.2705276933823120  3.8858565592802154 12.7278753470784327
  8.0906793446501606  5.3349940840367776  7.8262233893595337
  9.7802418007621341  5.3346950041145416 12.7303600940858423

Interface: ZnO(10-10)/fcc(111)_2sqrt3x2/Ag E_tot= -285.25359488 eV
 D3-zero damping= -18.9113925 eV, D3-BJ damping= -20.331445 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Ag
 1.0000000000000000
     9.9784384131079911    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7610541039000012    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.1021996581789182
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2  24
Selective dynamics
Cartesian
  3.3260644502799819  5.7556662109984709  8.9451241821253618   F   F   F
  1.6629934241335669  2.8751391792884893  8.0000001838787966   F   F   F
  3.3260649955109312  3.5714802856548644  8.9451248436730744   F   F   F
  1.6629925030996950  0.6909532505510081  8.0000000000000000   F   F   F
  1.6629960442343228  5.7556661319886882 11.7805090714841079   F   F   F
  3.3260711557905709  2.8751391002787066 10.8353850732375427   F   F   F
  1.6629965894652707  3.5714802066450821 11.7805097330318205   F   F   F
  3.3260702347566995  0.6909531715412253 10.8353848893587461   F   F   F
  3.3254026396772667  5.6614640480961063 14.4565906923584144   T   T   T
  1.6634007339589838  2.8128832936427561 13.6379125643199011   T   T   T
  3.3254025186726488  3.6060225582001313 14.4900683986863648   T   T   T
  1.6632892174443588  0.7209650654985265 13.6544163404645573   T   T   T
  1.6842593963928802  5.6840212870500526 17.0840570326395493   T   T   T
  3.3264626455798458  2.8576803070554861 16.3923178544006838   T   T   T
  1.6512922707503943  3.6895474662239147 17.1080531046376443   T   T   T
  3.3267885227362721  0.7798733316509153 16.3278313251365148   T   T   T
  6.6522105879826459  5.7556662109984709  8.9451241821253618   F   F   F
  4.9891395618362306  2.8751391792884893  8.0000001838787966   F   F   F
  6.6522111332135943  3.5714802856548644  8.9451248436730744   F   F   F
  4.9891386408023584  0.6909532505510081  8.0000000000000000   F   F   F
  4.9891421819369866  5.7556661319886882 11.7805090714841079   F   F   F
  6.6522172934932353  2.8751391002787066 10.8353850732375427   F   F   F
  4.9891427271679341  3.5714802066450821 11.7805097330318205   F   F   F
  6.6522163724593630  0.6909531715412253 10.8353848893587461   F   F   F
  6.6480461530910109  5.6485116870606742 14.4563527798557008   T   T   T
  4.9882078091738968  2.8073500173167645 13.6366649698632685   T   T   T
  6.6544394252268733  3.5956249514566272 14.4863445366095966   T   T   T
  4.9907418435875890  0.7183635320166357 13.6562250170350534   T   T   T
  4.9735166387007634  5.6828283221192342 17.0727222859394914   T   T   T
  6.6445492172678398  2.8106536299627494 16.3812507336702708   T   T   T
  5.0039644505962340  3.6915776147258583 17.0953314469131321   T   T   T
  6.6580193539637245  0.7458347366711107 16.3445378280503384   T   T   T
  9.9783567256853090  5.7556662109984709  8.9451241821253618   F   F   F
  8.3152856995388937  2.8751391792884893  8.0000001838787966   F   F   F
  9.9783572709162556  3.5714802856548644  8.9451248436730744   F   F   F
  8.3152847785050206  0.6909532505510081  8.0000000000000000   F   F   F
```

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  8.3152883196396505  5.7556661319886882 11.7805090714841079   F   F   F
  9.9783634311958984  2.8751391002787066 10.8353850732375427   F   F   F
  8.3152888648705972  3.5714802066450821 11.7805097330318205   F   F   F
  9.9783625101620270  0.6909531715412253 10.8353848893587461   F   F   F
  0.0046876227298798  5.6528043371511050 14.4517570749203319   T   T   T
  8.3155597937055141  2.8066006750747441 13.6361872502179189   T   T   T
  9.9765655622650957  3.5984351661946850 14.4880392896899881   T   T   T
  8.3140018702468339  0.7138154723441176 13.6613412102448262   T   T   T
  8.3246460477194830  5.6311374847194999 17.0283284785601126   T   T   T
  9.9879093554907872  2.8145669203130064 16.3842544837365907   T   T   T
  8.3148851256926513  3.6393130596552883 17.1158654994614068   T   T   T
  9.9835721142797258  0.7481829025762511 16.3422261270980336   T   T   T
  0.7135418903258371  1.1629506887771337 19.3667682063587279   T   T   T
  1.5982444339452682  2.6197575851994874 21.7117505632891081   T   T   T
  4.0946242317083774  1.1930763483970994 21.7390420724156606   T   T   T
  2.4153940545499064  1.1816714981324024 24.0750504748628629   T   T   T
  3.2441393025344070  2.5724445159249876 19.3483450784437352   T   T   T
  4.9203426508351944  2.6252008018498034 24.0983080766855835   T   T   T
  0.7719954795149495  4.0499464406846961 19.3685181521518643   T   T   T
  1.5815508038510799  5.4919435196497970 21.7324031613034414   T   T   T
  4.0775809121220998  4.0482811118723205 21.7242888481663847   T   T   T
  2.4206264280475982  4.0634102556988738 24.1082070959203953   T   T   T
  3.2551442742335142  5.5253379144379950 19.4276500472079761   T   T   T
  4.9017449631972374  5.5042345304835871 24.1170190797404693   T   T   T
  5.7767119138751175  1.1725211107879954 19.3768679182938079   T   T   T
  6.6010358958128847  2.6353615055810522 21.6914140606865509   T   T   T
  9.0839859635488054  1.2193282885566166 21.7698739810254942   T   T   T
  7.4003241096965375  1.1861135084685741 24.0969926782555959   T   T   T
  8.2521145652623833  2.6319345810566883 19.2713315557686684   T   T   T
  9.9110820640589363  2.6272346669462028 24.1421064651957025   T   T   T
  5.7235066719349899  4.0430837849874495 19.3665120755022002   T   T   T
  6.5441494440299932  5.4855542897399658 21.7877369991681675   T   T   T
  9.0954549378193850  4.0382430396890570 21.7554738455707941   T   T   T
  7.4139470799248057  4.0594698645947478 24.1233124688448086   T   T   T
  8.2215303932299104  5.5247435908182219 19.5863565914954094   T   T   T
  9.9014124589114143  5.5082329985924794 24.1047122250099228   T   T   T

Oxide reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Ag E_tot= -212.6009466 eV
 D3-zero damping= -7.5080583 eV, D3-BJ damping= -7.9204608 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     9.9784384131079911    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7610541039000012    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.3092812387561530
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2
Selective dynamics
Cartesian
  3.3260644502799819  5.7556662109984709  8.9451241821253618   F   F   F
  1.6629934241335669  2.8751391792884893  8.0000001838787966   F   F   F
  3.3260649955109312  3.5714802856548644  8.9451248436730744   F   F   F
  1.6629925030996950  0.6909532505510081  8.0000000000000000   F   F   F
  1.6629960442343228  5.7556661319886882 11.7805090714841079   F   F   F
  3.3260711557905709  2.8751391002787066 10.8353850732375427   F   F   F
  1.6629965894652707  3.5714802066450821 11.7805097330318205   F   F   F
  3.3260702347566995  0.6909531715412253 10.8353848893587461   F   F   F
  3.3259476372473231  5.6416960063581216 14.4330305888012997   T   T   T
  1.6619734899612273  2.8276383748681733 13.6537708285781321   T   T   T
  3.3254340471518726  3.5933979383185135 14.4819359406303647   T   T   T
  1.6635440688622676  0.7179502876360077 13.6596701482372751   T   T   T
  1.6639763202523177  5.4431079979351455 16.8314585831782892   T   T   T
  3.3264890110140075  2.7660725717872228 16.4521863738955005   T   T   T
  1.6647654638949851  3.5694630798965497 17.1020663218287510   T   T   T
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  3.3267385630408306  0.6711063324563301 16.3958051850187552   T   T   T
  6.6522105879826459  5.7556662109984709  8.9451241821253618   F   F   F
  4.9891395618362306  2.8751391792884893  8.0000001838787966   F   F   F
  6.6522111332135943  3.5714802856548644  8.9451248436730744   F   F   F
  4.9891386408023584  0.6909532505510081  8.0000000000000000   F   F   F
  4.9891421819369866  5.7556661319886882 11.7805090714841079   F   F   F
  6.6522172934932353  2.8751391002787066 10.8353850732375427   F   F   F
  4.9891427271679341  3.5714802066450821 11.7805097330318205   F   F   F
  6.6522163724593630  0.6909531715412253 10.8353848893587461   F   F   F
  6.6525380803834331  5.6417007342632344 14.4330583263175818   T   T   T
  4.9892260212950745  2.8233491910880182 13.6545120035877137   T   T   T
  6.6530045611267798  3.5933823794118647 14.4819680671619277   T   T   T
  4.9892360455188580  0.7171764464393104 13.6596950100346959   T   T   T
  4.9892544994468873  5.4437467668724597 16.8372447583910514   T   T   T
  6.6520747573583856  2.7660606216634660 16.4522473364297497   T   T   T
  4.9892716156823722  3.5686423083772745 17.0998102554094906   T   T   T
  6.6517953769266889  0.6711063880027709 16.3958443555003583   T   T   T
  9.9783567256853090  5.7556662109984709  8.9451241821253618   F   F   F
  8.3152856995388937  2.8751391792884893  8.0000001838787966   F   F   F
  9.9783572709162556  3.5714802856548644  8.9451248436730744   F   F   F
  8.3152847785050206  0.6909532505510081  8.0000000000000000   F   F   F
  8.3152883196396505  5.7556661319886882 11.7805090714841079   F   F   F
  9.9783634311958984  2.8751391002787066 10.8353850732375427   F   F   F
  8.3152888648705972  3.5714802066450821 11.7805097330318205   F   F   F
  9.9783625101620270  0.6909531715412253 10.8353848893587461   F   F   F
  0.0000040295258823  5.6434513983925942 14.4363352360058173   T   T   T
  8.3164700807875125  2.8276338838483177 13.6537579918612906   T   T   T
  9.9784349299164088  3.5944566724626679 14.4843475379478193   T   T   T
  8.3149551011539700  0.7179214865720250 13.6596891707015473   T   T   T
  8.3145209184899720  5.4431235820665549 16.8314426889397915   T   T   T
  9.9784680140043704  2.7683831690670799 16.4587253318494895   T   T   T
  8.3137846101134283  3.5694457746916668 17.1021051521695568   T   T   T
  9.9784748408789667  0.6715325374092175 16.3974531437171898   T   T   T

Metal reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Ag E_tot= -67.40199777 eV
 D3-zero damping= -7.674028 eV, D3-BJ damping= -9.7456828 eV
Ag
 1.0000000000000000
     9.9784384131079911    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7610541039000012    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.5552264120280803
  24
Cartesian
  0.5834640068799122  0.9790731445975438  7.9094029659373595
  1.3950039092336617  2.4145936308423113 10.2766944407194405
  3.8899687212434491  0.9759390500579469 10.2782348618292065
  2.2080902048205711  0.9809869901508439 12.6455210224616792
  3.0772049055941024  2.4187701866271256  7.9075116559442407
  4.7025091401677539  2.4229646509036034 12.6482869333488548
  0.5835182838084534  3.8594309690421951  7.9094547138898381
  1.3952813847108516  5.2951540859177078 10.2765737624526352
  3.8901400750845090  3.8573723317176771 10.2778898947191681
  2.2081175069738159  3.8617394762599671 12.6452701861444901
  3.0777657292300393  5.2994567328104134  7.9079197518441653
  4.7026789917408403  5.3034082559477715 12.6480651987570667
  5.5730781616417202  0.9789666062019340  7.9088615940796858
  6.3843787055365429  2.4137558209928476 10.2772703857627654
  8.8794086561850190  0.9761293254370645 10.2779241218947863
  7.1975283644512036  0.9806184844202674 12.6457121521684837
  8.0667445529064334  2.4191846229576255  7.9081253650870691
  9.6924599749878908  2.4227470792335870 12.6479786152573439
  5.5731140277324629  3.8594841845812446  7.9088141375328469
  6.3840607693707510  5.2941482968611098 10.2767773937733757
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  8.8797887070587578  3.8572524637920971 10.2782606973629118
  7.1974861733284943  3.8615568345529150 12.6458686821623658
  8.0664255920742800  5.2995284785198731  7.9082950176821223
  9.6921931796840024  5.3034642146601545 12.6476150063984338

Interface: ZnO(10-10)/fcc(111)_2sqrt3x2/Cu E_tot= -304.38877913 eV
 D3-zero damping= -18.9417841 eV, D3-BJ damping= -21.995283 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Cu
 1.0000000000000000
     8.7425944748320177    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.0475392734600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.1021996581789182
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2  24
Selective dynamics
Cartesian
  2.9141265879593559  5.0428186788376976  8.9451241821253618   F   F   F
  1.4570292985336637  2.5190490598409605  8.0000001838787966   F   F   F
  2.9141270656626688  3.1291473194163189  8.9451248436730744   F   F   F
  1.4570284915711604  0.6053776974460434  8.0000000000000000   F   F   F
  1.4570315941311753  5.0428186096133896 11.7805090714841079   F   F   F
  2.9141324629828214  2.5190489906166529 10.8353850732375427   F   F   F
  1.4570320718344869  3.1291472501920117 11.7805097330318205   F   F   F
  2.9141316560203188  0.6053776282217357 10.8353848893587461   F   F   F
  2.9096151962950270  5.1030554470032596 14.8620259764449454   T   T   T
  1.4558564079852900  2.5597232284949172 13.7055917783428178   T   T   T
  2.9108117202263522  3.1327411362378959 14.9069614812710309   T   T   T
  1.4515637213039403  0.6033196251061126 13.6721399394602514   T   T   T
  1.4665790984144689  5.1396340831609422 17.9781970072247361   T   T   T
  2.9034302134401950  2.5974927807402395 16.7942475929592625   T   T   T
  1.4513721392134784  3.1244871114377908 18.0382088794913855   T   T   T
  2.8910922550918450  0.6275690750339941 16.7187765423570269   T   T   T
  5.8283247462366949  5.0428186788376976  8.9451241821253618   F   F   F
  4.3712274568110026  2.5190490598409605  8.0000001838787966   F   F   F
  5.8283252239400074  3.1291473194163189  8.9451248436730744   F   F   F
  4.3712266498484995  0.6053776974460434  8.0000000000000000   F   F   F
  4.3712297524085137  5.0428186096133896 11.7805090714841079   F   F   F
  5.8283306212601609  2.5190489906166529 10.8353850732375427   F   F   F
  4.3712302301118253  3.1291472501920117 11.7805097330318205   F   F   F
  5.8283298142976578  0.6053776282217357 10.8353848893587461   F   F   F
  5.8186574816026804  5.1081231090234418 14.8764384458118961   T   T   T
  4.3667653767624062  2.5605784526219653 13.7055066244857269   T   T   T
  5.8256585679277846  3.1354037788330591 14.8978247771113033   T   T   T
  4.3676599758059966  0.6038162157585986 13.6742160235051173   T   T   T
  4.3152549632355024  5.1472343847181827 17.9739062388890964   T   T   T
  5.8117795218978152  2.6014574689164949 16.7852207519463406   T   T   T
  4.3641750806498782  3.1427768208452949 18.0071968565430289   T   T   T
  5.7859733149911996  0.6243449705728324 16.7461253769830201   T   T   T
  8.7425229045140345  5.0428186788376976  8.9451241821253618   F   F   F
  7.2854256150883412  2.5190490598409605  8.0000001838787966   F   F   F
  8.7425233822173443  3.1291473194163189  8.9451248436730744   F   F   F
  7.2854248081258381  0.6053776974460434  8.0000000000000000   F   F   F
  7.2854279106858542  5.0428186096133896 11.7805090714841079   F   F   F
  8.7425287795374995  2.5190489906166529 10.8353850732375427   F   F   F
  7.2854283883891648  3.1291472501920117 11.7805097330318205   F   F   F
  8.7425279725749974  0.6053776282217357 10.8353848893587461   F   F   F
 -0.0004192171150543  5.1025416115172835 14.8678425614498959   T   T   T
  7.2837173662462531  2.5574290895137510 13.7059541400413529   T   T   T
  8.7418349034640404  3.1307687444754739 14.9035446211300862   T   T   T
  7.2788298532975686  0.5991154364302066 13.6820305381599088   T   T   T
  7.2782496456493577  5.1633697430903709 17.9164322965089795   T   T   T
  8.7513984752522127  2.5945388526681143 16.7913514508708630   T   T   T
  7.2803818465181758  3.1484164447823342 17.9859118480548510   T   T   T
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  8.7580311677991904  0.6189659524649728 16.7351717786302601   T   T   T
  0.5997513270678166  1.0288936669720927 20.1025536222672621   T   T   T
  1.4079982424783821  2.3287511955359386 22.0712094141935147   T   T   T
  3.5696191843083804  1.0804732237018058 22.1280661712967159   T   T   T
  2.1198227783884924  1.0601679005058129 24.1733493711233720   T   T   T
  2.8183589205063346  2.2894050341868151 19.8884917750684842   T   T   T
  4.3166670772528963  2.3322427074883487 24.1827980350511780   T   T   T
  0.6759145062673665  3.5690329385974824 19.9835984519605354   T   T   T
  1.3802682002416835  4.8265975657000348 22.1253775369227164   T   T   T
  3.5704061459875760  3.5621600577732750 22.0693658127534498   T   T   T
  2.1278982120201992  3.5814030820833684 24.1912002543868319   T   T   T
  2.8327133520548138  4.8992145701262997 20.1096457322531883   T   T   T
  4.2952890621899344  4.8504085003975765 24.1989179559465164   T   T   T
  5.0394838517063620  1.0353135736941972 20.1259593532472287   T   T   T
  5.7877101356371359  2.3474996331756048 22.0643839420157377   T   T   T
  7.9451645220882332  1.0790116631460231 22.1506233466605984   T   T   T
  6.4849234693475468  1.0653828998626003 24.1905483098495502   T   T   T
  7.2080315552067784  2.2853400378157218 19.8546615563888196   T   T   T
  8.6913824316995569  2.3255807268962929 24.2178695252431488   T   T   T
  4.9813845650846673  3.5564780630571358 19.9716296738462979   T   T   T
  5.7309307796882196  4.8230643055100550 22.1731524929763069   T   T   T
  7.9767849178770422  3.5367524871853866 22.1135169725855611   T   T   T
  6.5053269399213791  3.5818703719148277 24.2102529033846920   T   T   T
  7.1821189694582754  4.8266919956367769 20.2502162505039074   T   T   T
  8.6763385923539111  4.8478334066673234 24.1915458323843247   T   T   T

Oxide reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Cu E_tot= -208.71587201 eV
 D3-zero damping= -8.6274097 eV, D3-BJ damping= -9.763438 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     8.7425944748320177    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.0475392734600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.3092812387561530
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2
Selective dynamics
Cartesian
  2.9141265879593559  5.0428186788376976  8.9451241821253618   F   F   F
  1.4570292985336637  2.5190490598409605  8.0000001838787966   F   F   F
  2.9141270656626688  3.1291473194163189  8.9451248436730744   F   F   F
  1.4570284915711604  0.6053776974460434  8.0000000000000000   F   F   F
  1.4570315941311753  5.0428186096133896 11.7805090714841079   F   F   F
  2.9141324629828214  2.5190489906166529 10.8353850732375427   F   F   F
  1.4570320718344869  3.1291472501920117 11.7805097330318205   F   F   F
  2.9141316560203188  0.6053776282217357 10.8353848893587461   F   F   F
  2.9145092032680946  5.0956421827972997 14.8368623833000743   T   T   T
  1.4574055070249583  2.5770553076058631 13.7218721642284134   T   T   T
  2.9145178603144046  3.1329909236615170 14.9220225793417196   T   T   T
  1.4574100316005223  0.6180441896771454 13.6696532255581289   T   T   T
  1.4568369799799024  4.8721633026058839 17.6976356448462404   T   T   T
  2.9143627562376784  2.5813600893547646 16.8601080189108821   T   T   T
  1.4573202780063634  3.0617950758766495 18.0563039041306581   T   T   T
  2.9139500925912682  0.6329455028396783 16.7262670023936941   T   T   T
  5.8283247462366949  5.0428186788376976  8.9451241821253618   F   F   F
  4.3712274568110026  2.5190490598409605  8.0000001838787966   F   F   F
  5.8283252239400074  3.1291473194163189  8.9451248436730744   F   F   F
  4.3712266498484995  0.6053776974460434  8.0000000000000000   F   F   F
  4.3712297524085137  5.0428186096133896 11.7805090714841079   F   F   F
  5.8283306212601609  2.5190489906166529 10.8353850732375427   F   F   F
  4.3712302301118253  3.1291472501920117 11.7805097330318205   F   F   F
  5.8283298142976578  0.6053776282217357 10.8353848893587461   F   F   F
  5.8287070137647738  5.0956302296851890 14.8368464728727325   T   T   T
  4.3715922593689243  2.5770568021401652 13.7218742060608694   T   T   T
```

```
  5.8287180783836723  3.1329810365827164 14.9220107737519321   T   T   T
  4.3716011581730605  0.6180447590239948 13.6696543601722755   T   T   T
  4.3710326828524737  4.8721513355655270 17.6976216383847564   T   T   T
  5.8285696572398562  2.5813433580947085 16.8600933557593216   T   T   T
  4.3715262739862366  3.0617834287774466 18.0562862854644877   T   T   T
  5.8281470489936318  0.6329297934640160 16.7262549723685936   T   T   T
  8.7425229045140345  5.0428186788376976  8.9451241821253618   F   F   F
  7.2854256150883412  2.5190490598409605  8.0000001838787966   F   F   F
  8.7425233822173443  3.1291473194163189  8.9451248436730744   F   F   F
  7.2854248081258381  0.6053776974460434  8.0000000000000000   F   F   F
  7.2854279106858542  5.0428186096133896 11.7805090714841079   F   F   F
  8.7425287795374995  2.5190489906166529 10.8353850732375427   F   F   F
  7.2854283883891648  3.1291472501920117 11.7805097330318205   F   F   F
  8.7425279725749974  0.6053776282217357 10.8353848893587461   F   F   F
  0.0003151055372162  5.0956352858040752 14.8368506448219488   T   T   T
  7.2857992191548142  2.5770549900342843 13.7218709796044003   T   T   T
  8.7429191619181061  3.1329863844341732 14.9220131699079097   T   T   T
  7.2858048731761356  0.6180433830906128 13.6696533833048708   T   T   T
  7.2852423432515190  4.8721541176051986 17.6976009442188555   T   T   T
  8.7427739550731367  2.5813614853224505 16.8600966787185804   T   T   T
  7.2857205340182203  3.0617891099657517 18.0562802848216357   T   T   T
  8.7423587473499573  0.6329471028036511 16.7262559813562532   T   T   T

Metal reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Cu E_tot= -89.6379499 eV
 D3-zero damping= -7.5131899 eV, D3-BJ damping= -9.4300403 eV
Cu
 1.0000000000000000
     8.7425944748320177    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.0475392734600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.5552264120280803
  24
Cartesian
  0.5037007097201616  0.8583298479541495  8.2042113155016949
  1.2201985740747205  2.1184393747667976 10.2773649698617415
  3.4057929111882723  0.8566640546989148 10.2779192257215115
  1.9439185947169231  0.8573195353361079 12.3507916116343068
  2.6888498189297008  2.1204018973132790  8.2043161788950627
  4.1298798095153213  2.1189613545286612 12.3507755570885447
  0.5037066538891679  3.3821597456503465  8.2041684726406743
  1.2204399911217620  4.6422320108588631 10.2775813593825038
  3.4058752163143313  3.3803532537927423 10.2778600930253123
  1.9437857569608745  3.3808929904849929 12.3507076226303596
  2.6887935675527599  4.6442096458700792  8.2044862896417481
  4.1300382379303278  4.6427855275609851 12.3506453616984455
  4.8748152968333480  0.8583304102987050  8.2043474592524444
  5.5919455361422630  2.1184368429639595 10.2775366993323765
  7.7778914097570944  0.8566553031608442 10.2780129928538990
  6.3156688219251942  0.8574260703724936 12.3506455596369342
  7.0607515672770180  2.1203255655097730  8.2045484575041616
  8.5010932744777570  2.1189665542062341 12.3507138882355409
  4.8749026139161602  3.3820510726422226  8.2042827366775288
  5.5920512442833346  4.6421902802579025 10.2776410292022202
  7.7779520056929634  3.3803759474757080 10.2779994744342762
  6.3154993265510839  3.3808103513431949 12.3506586722427496
  7.0608080091623293  4.6441855125538529  8.2045124620879886
  8.5011188603567334  4.6427854592172908 12.3506002044859500

Interface: ZnO(10-10)/fcc(111)_2sqrt3x2/Pt E_tot= -370.3898765 eV
 D3-zero damping= -23.7371062 eV, D3-BJ damping= -23.8984682 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Pt
 1.0000000000000000
     9.5971319778152502    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.5409067308400006    0.0000000000000000
```

```
     0.0000000000000000    0.0000000000000000   32.1021996581789182
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2  24
Selective dynamics
Cartesian
  3.1989654267068990  5.5357247256887341  8.9451241821253618   F   F   F
  1.5994453950513159  2.7652713797353203  8.0000001838787966   F   F   F
  3.1989659511029180  3.4350031777085537  8.9451248436730744   F   F   F
  1.5994445092129452  0.6645498284909550  8.0000000000000000   F   F   F
  1.5994479150300647  5.5357246496981549 11.7805090714841079   F   F   F
  3.1989718759795642  2.7652713037447412 10.8353850732375427   F   F   F
  1.5994484394260824  3.4350031017179750 11.7805097330318205   F   F   F
  3.1989709901411940  0.6645497525003760 10.8353848893587461   F   F   F
  3.1840637899014674  5.4971612966759942 14.6180330749293006   T   T   T
  1.6355507113171588  2.7179851059303304 13.6808582895885706   T   T   T
  3.1826221745742638  3.4816630294027191 14.7371866164221768   T   T   T
  1.6001442840619993  0.6932485492535686 13.6523088883523958   T   T   T
  1.5982898776706587  5.6762389537867657 17.4098666564635813   T   T   T
  3.1636034474410333  2.8538624276253142 16.7499993917558676   T   T   T
  1.4128250961484861  3.6477785577565771 17.3614347861166927   T   T   T
  3.1682726063895896  0.8509640249053149 16.4195123970742287   T   T   T
  6.3980094193119825  5.5357247256887341  8.9451241821253618   F   F   F
  4.7984893876563994  2.7652713797353203  8.0000001838787966   F   F   F
  6.3980099437080007  3.4350031777085537  8.9451248436730744   F   F   F
  4.7984885018180288  0.6645498284909550  8.0000000000000000   F   F   F
  4.7984919076351478  5.5357246496981549 11.7805090714841079   F   F   F
  6.3980158685846487  2.7652713037447412 10.8353850732375427   F   F   F
  4.7984924320311659  3.4350031017179750 11.7805097330318205   F   F   F
  6.3980149827462780  0.6645497525003760 10.8353848893587461   F   F   F
  6.3650541630140367  5.4286263172519487 14.5290613829291360   T   T   T
  4.7302090944505286  2.7206383909940830 13.6798833824106936   T   T   T
  6.3815020241959495  3.4239882026199240 14.5744227824399566   T   T   T
  4.7676304181462230  0.6950597086586672 13.6522615576810100   T   T   T
  4.7432205825024019  5.6801126344473545 17.3937828047472074   T   T   T
  6.3420313063180576  2.6311469859077223 16.4202588981799060   T   T   T
  4.9162597507775541  3.6538792841528935 17.3473380845347904   T   T   T
  6.3835217494686285  0.6515663434892907 16.3684698463330847   T   T   T
  9.5970534119170665  5.5357247256887341  8.9451241821253618   F   F   F
  7.9975333802614816  2.7652713797353203  8.0000001838787966   F   F   F
  9.5970539363130829  3.4350031777085537  8.9451248436730744   F   F   F
  7.9975324944231110  0.6645498284909550  8.0000000000000000   F   F   F
  7.9975359002402326  5.5357246496981549 11.7805090714841079   F   F   F
  9.5970598611897326  2.7652713037447412 10.8353850732375427   F   F   F
  7.9975364246362490  3.4350031017179750 11.7805097330318205   F   F   F
  9.5970589753513611  0.6645497525003760 10.8353848893587461   F   F   F
  0.0046318701401320  5.4249375707293606 14.5316620670507000   T   T   T
  7.9847598471583829  2.6743723268277217 13.6343969022172722   T   T   T
  9.5835050789787370  3.4210744343931045 14.5800864647728918   T   T   T
  7.9844094326824413  0.6615098200143057 13.6512560027505874   T   T   T
  7.9756246226075129  5.3905057549967861 17.2530085130554198   T   T   T
  9.5911976235590544  2.6278884085745173 16.4302954540392996   T   T   T
  7.9637961134703428  3.2863612827710180 17.3426815704586801   T   T   T
  9.5630001175129049  0.6489036418868350 16.3702488683283995   T   T   T
  0.7270850413881336  1.1250728136966943 19.6024381488220669   T   T   T
  1.5770648818461077  2.5407473975083503 21.9018844856838406   T   T   T
  3.9552509263569373  1.1511543942015852 21.9495585755579796   T   T   T
  2.3596954535186363  1.1907694479198043 24.2565751004410615   T   T   T
  3.1271296926567960  2.4394487826819837 19.6354142824559119   T   T   T
  4.7695286581388832  2.5776187162129673 24.1940352764064563   T   T   T
  0.7824706546385340  3.8380736914749272 19.4409874705991363   T   T   T
  1.5537419803211554  5.3239741522391055 21.9104350525950764   T   T   T
  3.9600105765698808  3.9110254827256825 21.8991150013455744   T   T   T
  2.3538112801014495  3.9627011440839879 24.2146737684393010   T   T   T
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  3.1244197894174537  5.2597380018158626 19.6407911404166740   T   T   T
  4.7614291327866622  5.3333109219826955 24.2057784848090733   T   T   T
  5.5195970029248826  1.1198915534598963 19.6022366505481891   T   T   T
  6.3812944787660495  2.5745464783345993 21.7707258851867707   T   T   T
  8.7388840227872819  1.2076014085846805 21.8404942740253709   T   T   T
  7.1534316896036936  1.2007221814928639 24.1420140267398864   T   T   T
  7.9190735946920237  2.6049311128282708 19.3483071001416036   T   T   T
  9.5524657045450336  2.5817168658377274 24.1328475684492680   T   T   T
  5.4542340979104029  3.8230106964444834 19.4334735667185114   T   T   T
  6.3198468814467246  5.3087914599944579 21.8658858512141343   T   T   T
  8.8152682264053581  3.9388093991838558 21.7681396203941802   T   T   T
  7.1730688809115239  3.9515638822645163 24.1033723607900612   T   T   T
  7.9154347092073589  5.3578153961438808 19.6955844890110257   T   T   T
  9.5530202923874121  5.3483684485358163 24.1667991153980672   T   T   T

Oxide reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Pt E_tot= -214.85120362 eV
 D3-zero damping= -7.743716 eV, D3-BJ damping= -8.4275601 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     9.5971319778152502    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.5409067308400006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.3092812387561530
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2
Selective dynamics
Cartesian
  3.1989654267068990  5.5357247256887341  8.9451241821253618   F   F   F
  1.5994453950513159  2.7652713797353203  8.0000001838787966   F   F   F
  3.1989659511029180  3.4350031777085537  8.9451248436730744   F   F   F
  1.5994445092129452  0.6645498284909550  8.0000000000000000   F   F   F
  1.5994479150300647  5.5357246496981549 11.7805090714841079   F   F   F
  3.1989718759795642  2.7652713037447412 10.8353850732375427   F   F   F
  1.5994484394260824  3.4350031017179750 11.7805097330318205   F   F   F
  3.1989709901411940  0.6645497525003760 10.8353848893587461   F   F   F
  3.1990494543816825  5.4395565434879991 14.5383217355527012   T   T   T
  1.5995135887667420  2.7198227813960014 13.6736010041510223   T   T   T
  3.1990412504586114  3.4386988108733938 14.6165688009769088   T   T   T
  1.5995320949426808  0.6869174376023748 13.6632261894348410   T   T   T
  1.5995290567394143  5.2288800477582216 17.0539301634785865   T   T   T
  3.1990771386436467  2.6621014340952631 16.5831013092138910   T   T   T
  1.5995400224314671  3.3960801839150099 17.3944620822326002   T   T   T
  3.1990654864467087  0.6480075449961633 16.4758777876289955   T   T   T
  6.3980094193119825  5.5357247256887341  8.9451241821253618   F   F   F
  4.7984893876563994  2.7652713797353203  8.0000001838787966   F   F   F
  6.3980099437080007  3.4350031777085537  8.9451248436730744   F   F   F
  4.7984885018180288  0.6645498284909550  8.0000000000000000   F   F   F
  4.7984919076351478  5.5357246496981549 11.7805090714841079   F   F   F
  6.3980158685846487  2.7652713037447412 10.8353850732375427   F   F   F
  4.7984924320311659  3.4350031017179750 11.7805097330318205   F   F   F
  6.3980149827462780  0.6645497525003760 10.8353848893587461   F   F   F
  6.3980878267693235  5.4395555591431979 14.5383425239614521   T   T   T
  4.7985615353272113  2.7198220645376425 13.6736024817531341   T   T   T
  6.3980827209197155  3.4386972717546200 14.6165816280673422   T   T   T
  4.7985809714779144  0.6869172213525484 13.6632266727058376   T   T   T
  4.7985703673557278  5.2288798219271344 17.0539680063031014   T   T   T
  6.3981188984827959  2.6620995547731137 16.5831208295383838   T   T   T
  4.7985810164497105  3.3960755008341938 17.3944824884725193   T   T   T
  6.3981050390588701  0.6480050663294145 16.4758957957826624   T   T   T
  9.5970534119170665  5.5357247256887341  8.9451241821253618   F   F   F
  7.9975333802614816  2.7652713797353203  8.0000001838787966   F   F   F
  9.5970539363130829  3.4350031777085537  8.9451248436730744   F   F   F
  7.9975324944231110  0.6645498284909550  8.0000000000000000   F   F   F
  7.9975359002402326  5.5357246496981549 11.7805090714841079   F   F   F
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  9.5970598611897326  2.7652713037447412 10.8353850732375427   F   F   F
  7.9975364246362490  3.4350031017179750 11.7805097330318205   F   F   F
  9.5970589753513611  0.6645497525003760 10.8353848893587461   F   F   F
 -0.0000030569026544  5.4395573794665362 14.5383192512737143   T   T   T
  7.9975948421467411  2.7198220430295308 13.6736022418103023   T   T   T
  9.5971254725813786  3.4386997233498215 14.6165660739656946   T   T   T
  7.9976129331654606  0.6869171041367782 13.6632270890644172   T   T   T
  7.9976225117024411  5.2288811174584264 17.0539611897549257   T   T   T
  9.5971622385129773  2.6621039583005244 16.5830973766790528   T   T   T
  7.9976313382173547  3.3960775125381115 17.3944780782070083   T   T   T
  9.5971459647500481  0.6480074029928765 16.4758752103260804   T   T   T

Metal reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Pt E_tot= -148.23589891 eV
 D3-zero damping= -11.5612319 eV, D3-BJ damping= -12.2927986 eV
Pt
 1.0000000000000000
     9.5971319778152502    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.5409067308400006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.5552264120280803
  24
Cartesian
  0.5147475183247928  0.9298443092341298  7.9646306644683955
  1.3424442700673724  2.3277210661590821 10.2782173144601234
  3.7410433658058397  0.9433564155506516 10.2777234160681505
  2.1701715194942142  0.9504280013892338 12.5921149585150616
  2.9143565456143374  2.3146139405865518  7.9647572924872199
  4.5698435413569820  2.3357748011322061 12.5910150854439333
  0.5148650572305152  3.7006942102817786  7.9648714861407157
  1.3417528254990094  5.0983475148745132 10.2783503895710826
  3.7412040975080449  3.7136463964134521 10.2781040643683905
  2.1703865902255783  3.7210798850904188 12.5921229980417468
  2.9145899794815060  5.0848186520674794  7.9649523341986503
  4.5699526632720113  5.1062308178295837 12.5911146193703551
  5.3138618112884943  0.9290231536133533  7.9640609020218056
  6.1399136736906819  2.3285986304093771 10.2768514342568356
  8.5393124777763649  0.9437606373650929 10.2773461391681984
  6.9683788290801258  0.9515617616516867 12.5896861136574660
  7.7129317822499219  2.3140417318351885  7.9636781087507389
  9.3675342737054077  2.3369456966432232 12.5907474827576458
  5.3134856377491619  3.6996839514571400  7.9638968771097511
  6.1402381379234479  5.0988712717779094 10.2767854456959817
  8.5391279878451165  3.7137948157105400 10.2771962404320121
  6.9685752514786898  3.7224805014234996 12.5897805696766927
  7.7125019121256067  5.0843815238689896  7.9636086001122104
  9.3675036022049856  5.1072319199061385 12.5907151077919952

Interface: ZnO(10-10)/fcc(111)_2sqrt3x2/Pd E_tot= -346.99444733 eV
 D3-zero damping= -20.5352139 eV, D3-BJ damping= -22.1879519 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Pd
 1.0000000000000000
     9.5192862237930260    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4959624638000006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.1021996581789182
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2  24
Selective dynamics
Cartesian
  3.1730174793087933  5.4908224917372941  8.9451241821253618   F   F   F
  1.5864717240542969  2.7428412791459800  8.0000001838787966   F   F   F
  3.1730179994512495  3.4071406440833432  8.9451248436730744   F   F   F
  1.5864708454012766  0.6591594282543216  8.0000000000000000   F   F   F
  1.5864742235926010  5.4908224163631019 11.7805090714841079   F   F   F
  3.1730238762691125  2.7428412037717878 10.8353850732375427   F   F   F
```

1.5864747437350559	3.4071405687091514	11.7805097330318205	F	F	F
3.1730229976160924	0.6591593528801291	10.8353848893587461	F	F	F
3.1607393289714367	5.4441516919145467	14.6258115846208625	T	T	T
1.5999881749610014	2.6928432804233808	13.6697518993113647	T	T	T
3.1604023119651763	3.4394135838885673	14.6928869689020676	T	T	T
1.5835473545411758	0.6796345830386665	13.6565477477633781	T	T	T
1.5929618627555127	5.5654211465265551	17.4556233623439603	T	T	T
3.1518115534412789	2.7916522062759199	16.6426308851378373	T	T	T
1.4889979498601582	3.5588418068208276	17.4022215196616052	T	T	T
3.1482688302456285	0.7928222836710302	16.4470899572074849	T	T	T
6.3461128872398023	5.4908224917372941	8.9451241821253618	F	F	F
4.7595671319853050	2.7428412791459800	8.0000001838787966	F	F	F
6.3461134073822576	3.4071406440833432	8.9451248436730744	F	F	F
4.7595662533322853	0.6591594282543216	8.0000000000000000	F	F	F
4.7595696315236093	5.4908224163631019	11.7805090714841079	F	F	F
6.3461192842001211	2.7428412037717878	10.8353850732375427	F	F	F
4.7595701516660647	3.4071405687091514	11.7805097330318205	F	F	F
6.3461184055471014	0.6591593528801291	10.8353848893587461	F	F	F
6.3188685919207401	5.3942948007919869	14.5741526217089774	T	T	T
4.7204412549080628	2.6945430377435162	13.6699035215763338	T	T	T
6.3339378245241313	3.3966474737158658	14.6145217851579279	T	T	T
4.7383190990266613	0.6804709384337675	13.6569270294591689	T	T	T
4.7024686017047150	5.5663866879817201	17.4469559100671070	T	T	T
6.3053174633371674	2.6394149564576952	16.4869903409886938	T	T	T
4.8173032902882120	3.5630251189588638	17.3889298015265581	T	T	T
6.3227675207898715	0.6565427549929459	16.4279234195779544	T	T	T
9.5192082951708112	5.4908224917372941	8.9451241821253618	F	F	F
7.9326625399163131	2.7428412791459800	8.0000001838787966	F	F	F
9.5192088153132648	3.4071406440833432	8.9451248436730744	F	F	F
7.9326616612632925	0.6591594282543216	8.0000000000000000	F	F	F
7.9326650394546192	5.4908224163631019	11.7805090714841079	F	F	F
9.5192146921311291	2.7428412037717878	10.8353850732375427	F	F	F
7.9326655595970728	3.4071405687091514	11.7805097330318205	F	F	F
9.5192138134781104	0.6591593528801291	10.8353848893587461	F	F	F
0.0028897100471797	5.3941347443615779	14.5752162622323986	T	T	T
7.9218642309754523	2.6667789671054871	13.6487354570521902	T	T	T
9.5083516140462336	3.3962640158248680	14.6179751265934073	T	T	T
7.9211715772333653	0.6568691838802989	13.6613441214702540	T	T	T
7.9131654716340716	5.3627434726150067	17.3046255216068623	T	T	T
9.5217061321150851	2.6394602786894019	16.4929712902886365	T	T	T
7.9108170992036690	3.3411397636854163	17.3909791139640717	T	T	T
9.5013800549344403	0.6567142648652156	16.4274399390668790	T	T	T
0.7070839494241760	1.1564814176469298	19.5984829835571013	T	T	T
1.5448653307989555	2.5329693802258744	21.8548235403128217	T	T	T
3.9106579759109845	1.1514639971210385	21.8699294377272402	T	T	T
2.3228903743603695	1.1623171477126097	24.1539810103055785	T	T	T
3.1097248546734724	2.4684153207245894	19.5823239468957837	T	T	T
4.7060223706170978	2.5363778440121227	24.1188061712977984	T	T	T
0.7724439360074229	3.8643499931967558	19.4897203195434940	T	T	T
1.5158221836738761	5.2854177679222794	21.8552303938146828	T	T	T
3.9095695673125386	3.8910211849683409	21.8549618533468895	T	T	T
2.3186723491000016	3.9138316373538533	24.1309826120416169	T	T	T
3.1129453669550022	5.2642775704483693	19.6278842788423127	T	T	T
4.6993861322294617	5.2819348842725660	24.1391433464899485	T	T	T
5.5105806688728656	1.1608651617498982	19.5982809781898482	T	T	T
6.3110064024587658	2.5447288893050084	21.8018105811713170	T	T	T
8.6596940461334899	1.1955417740215593	21.8503769483621255	T	T	T
7.0715683640140492	1.1637809711774572	24.1192659335965764	T	T	T
7.8732962427274398	2.5907841981845907	19.4100260978933470	T	T	T
9.4605222579740840	2.5405173345998415	24.1079212793447333	T	T	T
5.4432693848834894	3.8625488578604830	19.4782396268014431	T	T	T
6.2535404479313339	5.2653080065990059	21.8509314876603469	T	T	T
8.7026110170580502	3.9009082071519852	21.8163037008153786	T	T	T

```
  7.0856977275741615  3.9081885669295264 24.0935234370024816   T   T   T
  7.8644252064504796  5.3153781158112849 19.7358348673727981   T   T   T
  9.4559300946076110  5.2902840831776965 24.1292382159917054   T   T   T

Oxide reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Pd E_tot= -214.96351374 eV
 D3-zero damping= -7.8000723 eV, D3-BJ damping= -8.5399108 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     9.5192862237930260    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4959624638000006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.3092812387561530
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2
Selective dynamics
Cartesian
  3.1730174793087933  5.4908224917372941  8.9451241821253618   F   F   F
  1.5864717240542969  2.7428412791459800  8.0000001838787966   F   F   F
  3.1730179994512495  3.4071406440833432  8.9451248436730744   F   F   F
  1.5864708454012766  0.6591594282543216  8.0000000000000000   F   F   F
  1.5864742235926010  5.4908224163631019 11.7805090714841079   F   F   F
  3.1730238762691125  2.7428412037717878 10.8353850732375427   F   F   F
  1.5864747437350559  3.4071405687091514 11.7805097330318205   F   F   F
  3.1730229976160924  0.6591593528801291 10.8353848893587461   F   F   F
  3.1731305130618441  5.4030702782279247 14.5602201159423164   T   T   T
  1.5865788919076846  2.7005711248576323 13.6763104053388229   T   T   T
  3.1731269056959732  3.4091849724041867 14.6428366534682102   T   T   T
  1.5865752143592802  0.6802819606602536 13.6621011129910066   T   T   T
  1.5865928519918648  5.1909093200593821 17.0968939268857483   T   T   T
  3.1731766844760680  2.6516630195222683 16.6070819015895097   T   T   T
  1.5866163435691447  3.3667217801323259 17.4545172476864536   T   T   T
  3.1731587278375804  0.6479853957080847 16.4894671568478408   T   T   T
  6.3461128872398023  5.4908224917372941  8.9451241821253618   F   F   F
  4.7595671319853050  2.7428412791459800  8.0000001838787966   F   F   F
  6.3461134073822576  3.4071406440833432  8.9451248436730744   F   F   F
  4.7595662533322853  0.6591594282543216  8.0000000000000000   F   F   F
  4.7595696315236093  5.4908224163631019 11.7805090714841079   F   F   F
  6.3461192842001211  2.7428412037717878 10.8353850732375427   F   F   F
  4.7595701516660647  3.4071405687091514 11.7805097330318205   F   F   F
  6.3461184055471014  0.6591593528801291 10.8353848893587461   F   F   F
  6.3462212780312033  5.4030696359866877 14.5602383600474390   T   T   T
  4.7596790906193203  2.7005715493792830 13.6763117752733301   T   T   T
  6.3462193808581331  3.4091835471756187 14.6428502322818854   T   T   T
  4.7596748077652906  0.6802824279446231 13.6621020975782894   T   T   T
  4.7596932518958059  5.1909047426552730 17.0969031351614191   T   T   T
  6.3462681527937432  2.6516601245836759 16.6071053123124486   T   T   T
  4.7597090353091733  3.3667293432684438 17.4545362612371235   T   T   T
  6.3462484970713335  0.6479845061731084 16.4894787921344843   T   T   T
  9.5192082951708112  5.4908224917372941  8.9451241821253618   F   F   F
  7.9326625399163131  2.7428412791459800  8.0000001838787966   F   F   F
  9.5192088153132648  3.4071406440833432  8.9451248436730744   F   F   F
  7.9326616612632925  0.6591594282543216  8.0000000000000000   F   F   F
  7.9326650394546192  5.4908224163631019 11.7805090714841079   F   F   F
  9.5192146921311291  2.7428412037717878 10.8353850732375427   F   F   F
  7.9326655595970728  3.4071405687091514 11.7805097330318205   F   F   F
  9.5192138134781104  0.6591593528801291 10.8353848893587461   F   F   F
  0.0000282608776564  5.4030711753243645 14.5602212858277760   T   T   T
  7.9327626662521595  2.7005710020046170 13.6763114536239438   T   T   T
  9.5193132459271617  3.4091843196653238 14.6428336489315960   T   T   T
  7.9327600509624574  0.6802817848717893 13.6621023450533610   T   T   T
  7.9327977963851186  5.1909057370251919 17.0968978461850583   T   T   T
  9.5193609821010092  2.6516607603639453 16.6070777772089571   T   T   T
  7.9328112229732906  3.3667290968529202 17.4545319023737768   T   T   T
  9.5193520468716635  0.6479790886367092 16.4894686813659064   T   T   T
```

```
Metal reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Pd E_tot= -125.05645969 eV
 D3-zero damping= -8.7060611 eV, D3-BJ damping= -10.704265 eV
Pd
 1.0000000000000000
     9.5192862237930260    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4959624638000006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.5552264120280803
  24
Cartesian
  0.5142322940277891  0.9403326811682078  8.0006978726582663
  1.3339110513791863  2.3073708576332468 10.2772684175914701
  3.7136818667980043  0.9331929256223523 10.2777440440819010
  2.1456364446729994  0.9270666939126727 12.5545867868387013
  2.8939269129637806  2.3142667791567768  8.0008639503356829
  4.5253715611381553  2.3009654939223698 12.5548029005011497
  0.5142559534097616  3.6882431139572129  8.0006187405323708
  1.3341494931976610  5.0552840553050808 10.2774048374884739
  3.7138591332152386  3.6813613032567924 10.2778004990453091
  2.1455870488736779  3.6750094461634335 12.5544436714714962
  2.8941164347802562  5.0623394367277772  8.0014573300518332
  4.5253043801743136  5.0489937115523951 12.5545126305832380
  5.2736832530022619  0.9401713650461047  8.0008447136296965
  6.0937913016313736  2.3073499967783144 10.2774254445890847
  8.4742134699991940  0.9332108254256688 10.2773294770500723
  6.9055644603893782  0.9269288476962395 12.5544037849400869
  7.6539427481588449  2.3145460056628755  8.0008823373596574
  9.2851309696305879  2.3011014389246185 12.5544617412506376
  5.2738007181268909  3.6880410683825917  8.0007415546551677
  6.0938000561055130  5.0552675362467792 10.2772233293179820
  8.4742496542470303  3.6813960031284116 10.2773852500690701
  6.9055497860718704  3.6750279386302629 12.5543631860251992
  7.6540171932242362  5.0625960864874058  8.0007639387020912
  9.2850372733672657  5.0491292128484249 12.5543029045671712

Interface: ZnO(10-10)/fcc(111)_2sqrt3x2/Ni E_tot= -337.23085771 eV
 D3-zero damping= -17.4137441 eV, D3-BJ damping= -20.252645 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Ni
 1.0000000000000000
     8.5004137443782906    0.0000000000000000    0.0000000000000000
     0.0000000000000000    4.9077161635400008    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.0794358562141397
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2  24
Selective dynamics
Cartesian
  2.8334016603948546  4.9031263352545205  8.9451241821253618   F   F   F
  1.4166677764675102  2.4492682707265501  8.0000001838787966   F   F   F
  2.8334021248651924  3.0424660504068544  8.9451248436730744   F   F   F
  1.4166669918588710  0.5886079829877165  8.0000000000000000   F   F   F
  1.4166700084741184  4.9031262679478118 11.7805090714841079   F   F   F
  2.8334073726728701  2.4492682034198419 10.8353850732375427   F   F   F
  1.4166704729444546  3.0424659831001466 11.7805097330318205   F   F   F
  2.8334065880642312  0.5886079156810082 10.8353848893587461   F   F   F
  2.8348011327569398  5.0065997090244290 14.9448876094310013   T   T   T
  1.4215048132532184  2.5210108300435015 13.7223463106121422   T   T   T
  2.8332681084459357  3.0373773604873180 14.9951510657622240   T   T   T
  1.4168583203459366  0.5695357749019045 13.6797740938927888   T   T   T
  1.4570114301667789  5.0426011068198209 18.1390232454658111   T   T   T
  2.8379283265896191  2.5723866061312282 16.8914399101725259   T   T   T
  1.4111738759521892  3.0120722285921837 18.1973200957895500   T   T   T
  2.8378056710372501  0.6056692446637171 16.8035871200557487   T   T   T
  5.6668729085209515  4.9031263352545205  8.9451241821253618   F   F   F
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  4.2501390245936070  2.4492682707265501  8.0000001838787966   F   F   F
  5.6668733729912883  3.0424660504068544  8.9451248436730744   F   F   F
  4.2501382399849676  0.5886079829877165  8.0000000000000000   F   F   F
  4.2501412566002150  4.9031262679478118 11.7805090714841079   F   F   F
  5.6668786207989674  2.4492682034198419 10.8353850732375427   F   F   F
  4.2501417210705510  3.0424659831001466 11.7805097330318205   F   F   F
  5.6668778361903280  0.5886079156810082 10.8353848893587461   F   F   F
  5.6651557487921860  5.0018404667599530 14.9533210469331515   T   T   T
  4.2443347028427691  2.5220311888426346 13.7208016297218691   T   T   T
  5.6685265296690766  3.0308231723489896 14.9705141577071981   T   T   T
  4.2529230545602301  0.5708316737526046 13.6800629192720660   T   T   T
  4.2223377936504516  5.0544329240508503 18.1323342428410150   T   T   T
  5.6751227493581800  2.5506174096785426 16.8562358461010504   T   T   T
  4.2784053476272783  3.0358777490881459 18.1610285481312417   T   T   T
  5.6597789447333469  0.5741720826320720 16.8248253009889872   T   T   T
  8.5003441566470492  4.9031263352545205  8.9451241821253618   F   F   F
  7.0836102727197030  2.4492682707265501  8.0000001838787966   F   F   F
  8.5003446211173834  3.0424660504068544  8.9451248436730744   F   F   F
  7.0836094881110645  0.5886079829877165  8.0000000000000000   F   F   F
  7.0836125047263128  4.9031262679478118 11.7805090714841079   F   F   F
  8.5003498689250652  2.4492682034198419 10.8353850732375427   F   F   F
  7.0836129691966478  3.0424659831001466 11.7805097330318205   F   F   F
  8.5003490843164258  0.5886079156810082 10.8353848893587461   F   F   F
  0.0040271742026509  4.9956149157818981 14.9508880394587944   T   T   T
  7.0861801026403333  2.5123751154610487 13.7151986043069449   T   T   T
  8.5007566466966153  3.0242665286131349 14.9813843019908095   T   T   T
  7.0857815246323703  0.5610650327667870 13.6858361089225706   T   T   T
  7.0995137822616643  5.0733379941583108 18.1029646221205134   T   T   T
  8.5178366053978110  2.5411761610401240 16.8688060901048047   T   T   T
  7.0930095146387213  3.0075994576209566 18.1587058516636546   T   T   T
  8.5331367260328310  0.5644088753729702 16.8221935622441983   T   T   T
  0.6209578090507566  0.8810533011411795 20.2746920881838300   T   T   T
  1.4094461060656307  2.1244885961337516 22.1780840627359801   T   T   T
  3.5210664803344560  0.9090854542746227 22.2023138597007588   T   T   T
  2.1062638458737961  0.8951255224840737 24.1958362893342809   T   T   T
  2.7910808996938177  2.0923265347444047 20.1067266806727147   T   T   T
  4.2430517666791925  2.1275485863017369 24.1863805101443390   T   T   T
  0.7177668414965341  3.3306145023173541 20.0830096748078191   T   T   T
  1.3833571779138070  4.5569871268784139 22.2008177370621382   T   T   T
  3.5311322415113948  3.3392922181170803 22.1649312515279568   T   T   T
  2.1140909634747160  3.3486055773733701 24.1923873695599347   T   T   T
  2.7966028610026590  4.6172676249658249 20.2424271945160221   T   T   T
  4.2213604816349211  4.5743579838819191 24.2141657988468992   T   T   T
  4.9599096048441060  0.8742908229188809 20.2882891387336173   T   T   T
  5.6786872946959566  2.1469762873733362 22.1525479315001199   T   T   T
  7.7485371561317322  0.9141834190899433 22.2253772386377868   T   T   T
  6.3501551894235853  0.8969727715076703 24.2181708712581489   T   T   T
  7.0508691257892178  2.1316790361007656 19.9475719027893312   T   T   T
  8.4967890004112157  2.1174920906800843 24.2155236894017136   T   T   T
  4.8782004547343085  3.3158119303799229 20.0593481797756610   T   T   T
  5.6253128209894525  4.5471948547746264 22.2443625347402900   T   T   T
  7.8058261211993365  3.3132675527878344 22.1803756515652566   T   T   T
  6.3717889608305960  3.3411643823512316 24.2112723095120899   T   T   T
  7.0361480200513187  4.5575837015295599 20.3638925074994184   T   T   T
  8.4845950603558347  4.5701403051639033 24.2059706915955388   T   T   T

Oxide reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Ni E_tot= -203.49045032 eV
 D3-zero damping= -9.0122975 eV, D3-BJ damping= -10.2171051 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     8.5004137443782906    0.0000000000000000    0.0000000000000000
     0.0000000000000000    4.9077161635400008    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.3092812387561530
```

```
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2
Selective dynamics
Cartesian
  2.8334016603948546  4.9031263352545205  8.9451241821253618   F   F   F
  1.4166677764675102  2.4492682707265501  8.0000001838787966   F   F   F
  2.8334021248651924  3.0424660504068544  8.9451248436730744   F   F   F
  1.4166669918588710  0.5886079829877165  8.0000000000000000   F   F   F
  1.4166700084741184  4.9031262679478118 11.7805090714841079   F   F   F
  2.8334073726728701  2.4492682034198419 10.8353850732375427   F   F   F
  1.4166704729444546  3.0424659831001466 11.7805097330318205   F   F   F
  2.8334065880642312  0.5886079156810082 10.8353848893587461   F   F   F
  2.8320369904788461  4.9828278852347214 14.9262148408664270   T   T   T
  1.4153186928667401  2.5251436945479679 13.7319050303654322   T   T   T
  2.8320041401892091  3.0216919411473286 14.9971018632223032   T   T   T
  1.4152717958455234  0.5726522192715491 13.6785974014951748   T   T   T
  1.4153813831810234  4.7835359036598097 17.9098179018365791   T   T   T
  2.8327856507122209  2.5470908767765232 16.9319468191017890   T   T   T
  1.4159306832755716  2.9551184295517849 18.2136561205069576   T   T   T
  2.8321028215684083  0.6016830843475029 16.8125618921232949   T   T   T
  5.6668729085209515  4.9031263352545205  8.9451241821253618   F   F   F
  4.2501390245936070  2.4492682707265501  8.0000001838787966   F   F   F
  5.6668733729912883  3.0424660504068544  8.9451248436730744   F   F   F
  4.2501382399849676  0.5886079829877165  8.0000000000000000   F   F   F
  4.2501412566002150  4.9031262679478118 11.7805090714841079   F   F   F
  5.6668786207989674  2.4492682034198419 10.8353850732375427   F   F   F
  4.2501417210705510  3.0424659831001466 11.7805097330318205   F   F   F
  5.6668778361903280  0.5886079156810082 10.8353848893587461   F   F   F
  5.6655070491445390  4.9827663003545810 14.9261124242206034   T   T   T
  4.2487591255354342  2.5252205615426648 13.7319022595925624   T   T   T
  5.6654922080943271  3.0216459623694143 14.9970308027773171   T   T   T
  4.2487385494549406  0.5727364441026359 13.6785930521132979   T   T   T
  4.2488547577952573  4.7836513731555463 17.9099031388614911   T   T   T
  5.6661725739465076  2.5470139044154632 16.9318469220363212   T   T   T
  4.2494459854420548  2.9551928829664038 18.2136170731491163   T   T   T
  5.6655393702990953  0.6016417746490323 16.8124734160309188   T   T   T
  8.5003441566470492  4.9031263352545205  8.9451241821253618   F   F   F
  7.0836102727197030  2.4492682707265501  8.0000001838787966   F   F   F
  8.5003446211173834  3.0424660504068544  8.9451248436730744   F   F   F
  7.0836094881110645  0.5886079829877165  8.0000000000000000   F   F   F
  7.0836125047263128  4.9031262679478118 11.7805090714841079   F   F   F
  8.5003498689250652  2.4492682034198419 10.8353850732375427   F   F   F
  7.0836129691966478  3.0424659831001466 11.7805097330318205   F   F   F
  8.5003490843164258  0.5886079156810082 10.8353848893587461   F   F   F
 -0.0014611271207718  4.9827510946788207 14.9261331701607318   T   T   T
  7.0822778641401545  2.5252291755782648 13.7318632561305733   T   T   T
  8.4989773874056684  3.0216136223407886 14.9970434313320755   T   T   T
  7.0822101598168148  0.5727527705697043 13.6785490322346099   T   T   T
  7.0823219830589572  4.7835973105144012 17.9097309440940720   T   T   T
  8.4997760375421478  2.5469956481187399 16.9318462971249559   T   T   T
  7.0829006756100421  2.9551453039954358 18.2134296109870100   T   T   T
  8.4990551939560355  0.6015904275587964 16.8124805118113869   T   T   T

Metal reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Ni E_tot= -127.00137741 eV
 D3-zero damping= -5.8932798 eV, D3-BJ damping= -7.4891375 eV
Ni
 1.0000000000000000
     8.5004137443782906    0.0000000000000000    0.0000000000000000
     0.0000000000000000    4.9077161635400008    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.5552264120280803
  24
Cartesian
  0.4705045234986113  0.8376666303220234  8.2694593154404519
```

```
  1.1880004761789362  2.0649392524590673 10.2763857583544702
  3.3157530962446953  0.8359403945331144 10.2795135897973005
  1.9048880855651580  0.8274599111671572 12.2843784486276100
  2.5977822888957247  2.0635062734720608  8.2709198435740543
  4.0317428942346094  2.0528743488072858 12.2842677036312580
  0.4707573413838656  3.2914720643572712  8.2698392332170165
  1.1881075884295547  4.5185501593002781 10.2759157616979451
  3.3153679552638358  3.2898831220773053 10.2796412848516852
  1.9048873393468759  3.2815363491045906 12.2848169088335482
  2.5978673123595866  4.5177091752700171  8.2706969397890902
  4.0318067001715541  4.5067582122046179 12.2845189755687230
  4.7212081754404460  0.8379768356598341  8.2695809026367826
  5.4378804154500315  2.0648373262300095 10.2764206700222562
  7.5656136090733908  0.8359651483951114 10.2793477623270171
  6.1550004694147562  0.8274294376550031 12.2846081687997106
  6.8476405287657247  2.0639875301214219  8.2714819099779646
  8.2823216845649750  2.0529151140101436 12.2840448291847189
  4.7209282542701629  3.2918326159041547  8.2698983819753593
  5.4379568601284891  4.5186146737796102 10.2764608443252694
  7.5656938316339186  3.2896682957709795 10.2795575026768944
  6.1550372940155524  3.2811441402349688 12.2846424784157300
  6.8481798812427206  4.5175109449952942  8.2716428575123118
  8.2819991611799875  4.5066801323832948 12.2842897867490723

Interface: ZnO(10-10)/fcc(111)_2sqrt3x2/Ir E_tot= -430.54095982 eV
 D3-zero damping= -22.6149229 eV, D3-BJ damping= -23.3887526 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Ir
 1.0000000000000000
     9.4052548667237605    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4301264291000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.1021996581789182
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2  24
Selective dynamics
Cartesian
  3.1350079604579242  5.4250480286694351  8.9451241821253618   F   F   F
  1.5674674080380648  2.7099848331968222  8.0000001838787966   F   F   F
  3.1350084743696036  3.3663265680868064  8.9451248436730744   F   F   F
  1.5674665399104131  0.6512633694152701  8.0000000000000000   F   F   F
  1.5674698776344449  5.4250479541981491 11.7805090714841079   F   F   F
  3.1350142807891714  2.7099847587255361 10.8353850732375427   F   F   F
  1.5674703915461228  3.3663264936155204 11.7805097330318205   F   F   F
  3.1350134126615203  0.6512632949439837 10.8353848893587461   F   F   F
  3.1190082948383129  5.4291394247317051 14.6764196169817698   T   T   T
  1.5994123862219400  2.6890624916528472 13.6933030212747280   T   T   T
  3.1224582626770321  3.4264902735246388 14.7917394000906288   T   T   T
  1.5705006925175360  0.6879190877417602 13.6487880834864868   T   T   T
  1.5642834138659529  5.5800775912212881 17.5313591602336274   T   T   T
  3.1122155635652473  2.8366761878808342 16.7674188403527964   T   T   T
  1.3920532737603128  3.5555887265885180 17.5345371316280350   T   T   T
  3.1090149734960706  0.8436052865257018 16.4790381157266381   T   T   T
  6.2700929160325112  5.4250480286694351  8.9451241821253618   F   F   F
  4.7025523636126518  2.7099848331968222  8.0000001838787966   F   F   F
  6.2700934299441897  3.3663265680868064  8.9451248436730744   F   F   F
  4.7025514954850003  0.6512633694152701  8.0000000000000000   F   F   F
  4.7025548332090317  5.4250479541981491 11.7805090714841079   F   F   F
  6.2700992363637589  2.7099847587255361 10.8353850732375427   F   F   F
  4.7025553471207093  3.3663264936155204 11.7805097330318205   F   F   F
  6.2700983682361073  0.6512632949439837 10.8353848893587461   F   F   F
  6.2326617208729607  5.3441520772112856 14.5824162527058387   T   T   T
  4.6470965841494793  2.6893543267639930 13.6937571872044437   T   T   T
  6.2591652016511219  3.3528659849355931 14.6637463646951147   T   T   T
  4.6704050977651574  0.6878771919110981 13.6499845972574700   T   T   T
```

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  4.6564937965619810  5.5903145573799602 17.5250075911301728   T   T   T
  6.2267654484398909  2.6051328439409476 16.5229043877091222   T   T   T
  4.8293830129245938  3.5671689069539716 17.5360489105627835   T   T   T
  6.2436028358918865  0.6309805829606083 16.4263621819339676   T   T   T
  9.4051778716070977  5.4250480286694351  8.9451241821253618   F   F   F
  7.8376373191872375  2.7099848331968222  8.0000001838787966   F   F   F
  9.4051783855187754  3.3663265680868064  8.9451248436730744   F   F   F
  7.8376364510595860  0.6512633694152701  8.0000000000000000   F   F   F
  7.8376397887836200  5.4250479541981491 11.7805090714841079   F   F   F
  9.4051841919383463  2.7099847587255361 10.8353850732375427   F   F   F
  7.8376403026952968  3.3663264936155204 11.7805097330318205   F   F   F
  9.4051833238106948  0.6512632949439837 10.8353848893587461   F   F   F
  0.0096284523140996  5.3424401762145886 14.5803917380800829   T   T   T
  7.8231208381704622  2.6434849955939419 13.6500338844583204   T   T   T
  9.3897551812862385  3.3510540681633194 14.6609426244073919   T   T   T
  7.8236576276740877  0.6479200220180861 13.6540009208099793   T   T   T
  7.8177169047783019  5.2864571314718480 17.3499497813233106   T   T   T
  9.3983518449894952  2.6007344940349393 16.5195098169846659   T   T   T
  7.8134529525496639  3.1714289236350104 17.5478759099369661   T   T   T
  9.3888774839370512  0.6263164186646107 16.4259662123620558   T   T   T
  0.7310069009740288  1.1776990865630972 19.7605776234065900   T   T   T
  1.5128033296804033  2.5391818766007797 21.9297128263925885   T   T   T
  3.8927772335023625  1.1782655329256377 21.9505232542829809   T   T   T
  2.2976341329174690  1.1801997475986743 24.0857348321574385   T   T   T
  3.0931354631039918  2.5089514856389883 19.7994043102188115   T   T   T
  4.6761805410308819  2.5387076312868810 24.0882080888094521   T   T   T
  0.7965884308688549  3.8533776039840593 19.6630736662278487   T   T   T
  1.5097857085942068  5.2407625415904722 21.9025698528997239   T   T   T
  3.8816295279654298  3.8946063007088667 21.9191186822049993   T   T   T
  2.3115619076748506  3.9034808831217664 24.0843431223796358   T   T   T
  3.0964665709946142  5.2755698258501971 19.7616470156933985   T   T   T
  4.6561189873611326  5.2496608714323232 24.1055735575837780   T   T   T
  5.4482425059977535  1.1666265718804334 19.7685254259905570   T   T   T
  6.2516097352191844  2.5545981704643510 21.8666367353807800   T   T   T
  8.5664131840367599  1.2156352096167238 21.9018815067717796   T   T   T
  7.0078548889531254  1.1921724732664174 24.0808130549756889   T   T   T
  7.8027848511284770  2.5961765069952873 19.6015290987879141   T   T   T
  9.3602755574107182  2.5386465545373773 24.0924300144482935   T   T   T
  5.3900945476977249  3.8543609007440098 19.6608069222869766   T   T   T
  6.2249484972961273  5.2300032096672924 21.9032866789022229   T   T   T
  8.5903258850564281  3.8944417087908318 21.8577469586032151   T   T   T
  7.0103995883714658  3.9003574638957641 24.0835291005441015   T   T   T
  7.7889612765479361  5.3025428266115480 19.8047224386498009   T   T   T
  9.3461645820036008  5.2467941772618190 24.0661514040757254   T   T   T

Oxide reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Ir E_tot= -214.9068046 eV
 D3-zero damping= -7.8857129 eV, D3-BJ damping= -8.7008397 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     9.4052548667237605    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4301264291000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.3092812387561530
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2
Selective dynamics
Cartesian
  3.1350079604579242  5.4250480286694351  8.9451241821253618   F   F   F
  1.5674674080380648  2.7099848331968222  8.0000001838787966   F   F   F
  3.1350084743696036  3.3663265680868064  8.9451248436730744   F   F   F
  1.5674665399104131  0.6512633694152701  8.0000000000000000   F   F   F
  1.5674698776344449  5.4250479541981491 11.7805090714841079   F   F   F
  3.1350142807891714  2.7099847587255361 10.8353850732375427   F   F   F
  1.5674703915461228  3.3663264936155204 11.7805097330318205   F   F   F
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  3.1350134126615203  0.6512632949439837 10.8353848893587461   F   F   F
  3.1350709931221781  5.3490763734552074 14.5969609981752875   T   T   T
  1.5675355670097941  2.6747312430913208 13.6827403013680975   T   T   T
  3.1350762162776800  3.3629333268961976 14.6853689205635067   T   T   T
  1.5675421057518240  0.6687100174830233 13.6626299730827085   T   T   T
  1.5676848570319273  5.1348423845195592 17.1774058471829605   T   T   T
  3.1351001777077130  2.6334705933438971 16.6483401336712227   T   T   T
  1.5675476054583564  3.3183741099319124 17.5497453099248695   T   T   T
  3.1352096897484207  0.6423960077425880 16.5190399501606926   T   T   T
  6.2700929160325112  5.4250480286694351  8.9451241821253618   F   F   F
  4.7025523636126518  2.7099848331968222  8.0000001838787966   F   F   F
  6.2700934299441897  3.3663265680868064  8.9451248436730744   F   F   F
  4.7025514954850003  0.6512633694152701  8.0000000000000000   F   F   F
  4.7025548332090317  5.4250479541981491 11.7805090714841079   F   F   F
  6.2700992363637589  2.7099847587255361 10.8353850732375427   F   F   F
  4.7025553471207093  3.3663264936155204 11.7805097330318205   F   F   F
  6.2700983682361073  0.6512632949439837 10.8353848893587461   F   F   F
  6.2701828103765207  5.3490726475265395 14.5969110697581108   T   T   T
  4.7026124306330779  2.6747267435868509 13.6827397582026933   T   T   T
  6.2701596162398516  3.3629271476582523 14.6853639532109881   T   T   T
  4.7026248114143190  0.6687079264435002 13.6626265306406296   T   T   T
  4.7027875585624948  5.1348375521754965 17.1773908977973377   T   T   T
  6.2701800997283277  2.6334615568579434 16.6483290336857834   T   T   T
  4.7026400756303994  3.3183743497146967 17.5497512135320122   T   T   T
  6.2702912531192947  0.6423951609921849 16.5189951389110021   T   T   T
  9.4051778716070977  5.4250480286694351  8.9451241821253618   F   F   F
  7.8376373191872375  2.7099848331968222  8.0000001838787966   F   F   F
  9.4051783855187754  3.3663265680868064  8.9451248436730744   F   F   F
  7.8376364510595860  0.6512633694152701  8.0000000000000000   F   F   F
  7.8376397887836200  5.4250479541981491 11.7805090714841079   F   F   F
  9.4051841919383463  2.7099847587255361 10.8353850732375427   F   F   F
  7.8376403026952968  3.3663264936155204 11.7805097330318205   F   F   F
  9.4051833238106948  0.6512632949439837 10.8353848893587461   F   F   F
 -0.0000077991233403  5.3490755876477323 14.5969544549387376   T   T   T
  7.8377058209700952  2.6747283425002495 13.6827383976838171   T   T   T
  9.4052436359214582  3.3629337651132096 14.6853681341416085   T   T   T
  7.8377267336737884  0.6687122659615604 13.6626184372267740   T   T   T
  7.8378456890683506  5.1348399221139189 17.1773843814456129   T   T   T
  9.4052618374178358  2.6334742211569218 16.6483328793480929   T   T   T
  7.8377140681078421  3.3183774701947040 17.5497460076574008   T   T   T
  9.4053730471226782  0.6423993011015217 16.5190308234368430   T   T   T

Metal reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Ir E_tot= -208.40079382 eV
 D3-zero damping= -10.6763283 eV, D3-BJ damping= -11.6304695 eV
Ir
 1.0000000000000000
     9.4052548667237605    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4301264291000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.5552264120280803
  24
Cartesian
  0.5323885238573127  0.9224258137998483  8.1055196013095188
  1.3151122714593826  2.2794889853126681 10.2776814698577663
  3.6662754724242719  0.9220563672486355 10.2776567551687368
  2.0987206754253491  0.9228090807267487 12.4495710200723853
  2.8834803401348026  2.2798974620105987  8.1054721642972911
  4.4503620393067189  2.2802813591194178 12.4496772876743620
  0.5324033738343957  3.6375390127371596  8.1055277526364424
  1.3151026671738608  4.9945927149170402 10.2776799366335538
  3.6662851121089561  3.6369287205777643 10.2776327159389265
  2.0987147237873307  3.6377640515913421 12.4495673777300198
  2.8834649739141227  4.9949866133459553  8.1054430818283691
  4.4503369915193627  4.9953306348146462 12.4497002265264474
```

```
  5.2349459675746628  0.9224403353036651  8.1054078460259333
  6.0178980915267886  2.2794877735662888 10.2778363917334232
  8.3691945816446527  0.9220500240923876 10.2778065872736750
  6.8014185507057308  0.9228451326567511 12.4495132265668627
  7.5862043538791442  2.2798893268669862  8.1054497611846372
  9.1528748331914294  2.2803256447657447 12.4495635808565144
  5.2349243097320413  3.6374460616391633  8.1053913572086742
  6.0178942055816780  4.9945494069295062 10.2778067887280269
  8.3692094520167934  3.6369828360690986 10.2778114533012612
  6.8014134673628019  3.6377805482909462 12.4495485874749860
  7.5862223380670457  4.9949764478476943  8.1054481657998210
  9.1529141943984680  4.9954002161686235 12.4496137754019038

Interface: ZnO(10-10)/fcc(111)_2sqrt3x2/Rh E_tot= -392.48987005 eV
 D3-zero damping= -20.6582633 eV, D3-BJ damping= -22.2357483 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Rh
 1.0000000000000000
     9.2756956675135616    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3553253905600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.1021996581789182
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2  24
Selective dynamics
Cartesian
  3.0918226213437685  5.3503169460745283  8.9451241821253618   F   F   F
  1.5458752422699680  2.6726542696091213  8.0000001838787966   F   F   F
  3.0918231281762156  3.3199547705521724  8.9451248436730744   F   F   F
  1.5458743861009421  0.6422920909319076  8.0000000000000000   F   F   F
  1.5458776778471819  5.3503168726290991 11.7805090714841079   F   F   F
  3.0918288546112342  2.6726541961636912 10.8353850732375427   F   F   F
  1.5458781846796272  3.3199546971067431 11.7805097330318205   F   F   F
  3.0918279984422088  0.6422920174864777 10.8353848893587461   F   F   F
  3.0831340692424933  5.3347815492202875 14.6978391623670568   T   T   T
  1.5641523592117241  2.6463074828404021 13.6898722086853422   T   T   T
  3.0850544496919237  3.3455320631887675 14.7870266538771915   T   T   T
  1.5478432420880270  0.6580173271394196 13.6559812682126154   T   T   T
  1.5537064500810533  5.4494784854572504 17.6188271408795707   T   T   T
  3.0776665763820432  2.7382562563081740 16.7238226514471719   T   T   T
  1.4482643308589518  3.4288407543850203 17.6353153191652936   T   T   T
  3.0682596022888182  0.7584888332189295 16.5171342641071597   T   T   T
  6.1837211771816225  5.3503169460745283  8.9451241821253618   F   F   F
  4.6377737981078218  2.6726542696091213  8.0000001838787966   F   F   F
  6.1837216840140687  3.3199547705521724  8.9451248436730744   F   F   F
  4.6377729419387963  0.6422920909319076  8.0000000000000000   F   F   F
  4.6377762336850354  5.3503168726290991 11.7805090714841079   F   F   F
  6.1837274104490891  2.6726541961636912 10.8353850732375427   F   F   F
  4.6377767405174808  3.3199546971067431 11.7805097330318205   F   F   F
  6.1837265542800628  0.6422920174864777 10.8353848893587461   F   F   F
  6.1571672619976470  5.2778281868454533 14.6453195339929323   T   T   T
  4.6052086205362635  2.6465173517731402 13.6881558148485052   T   T   T
  6.1789458227024534  3.2940285162434528 14.7123190480360506   T   T   T
  4.6185463970439828  0.6581907220999397 13.6560921384615046   T   T   T
  4.5827784009990662  5.4495159831372098 17.6090099595403622   T   T   T
  6.1511864186027099  2.5814211365286739 16.5855642045794980   T   T   T
  4.7094303654338869  3.4377331460281062 17.6094022336311333   T   T   T
  6.1507174655341643  0.6103367019990583 16.4989981013889349   T   T   T
  9.2756197330194770  5.3503169460745283  8.9451241821253618   F   F   F
  7.7296723539456753  2.6726542696091213  8.0000001838787966   F   F   F
  9.2756202398519214  3.3199547705521724  8.9451248436730744   F   F   F
  7.7296714977766490  0.6422920909319076  8.0000000000000000   F   F   F
  7.7296747895228908  5.3503168726290991 11.7805090714841079   F   F   F
  9.2756259662869436  2.6726541961636912 10.8353850732375427   F   F   F
  7.7296752963553352  3.3199546971067431 11.7805097330318205   F   F   F
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```
  9.2756251101179163  0.6422920174864777 10.8353848893587461   F   F   F
  0.0102476196085072  5.2769552252209504 14.6460226560589533   T   T   T
  7.7255992213750604  2.6153753999493117 13.6658707892567968   T   T   T
  9.2691036009827048  3.2927730684946535 14.7208475702509922   T   T   T
  7.7224431231163315  0.6282269211720116 13.6647328221283377   T   T   T
  7.7111388891479455  5.2366902648615863 17.4583040778841578   T   T   T
  9.2829863050322903  2.5820473708400340 16.5980676579038651   T   T   T
  7.7103253922876460  3.1911073120079734 17.6121426098088847   T   T   T
  9.2719606957941085  0.6086741931340034 16.5008210240701239   T   T   T
  0.6794197447459238  1.1402079906115368 19.8108499718084836   T   T   T
  1.4679331521747219  2.4806193471524067 21.9435138282175153   T   T   T
  3.7964850126241516  1.1322818072945420 21.9444463400511829   T   T   T
  2.2314157934769070  1.1324296401894920 24.0799952661188499   T   T   T
  3.0135186515241248  2.4440315548167866 19.8034572506403421   T   T   T
  4.5662211200990956  2.4664827339626689 24.0789205382383358   T   T   T
  0.7391372401310244  3.7786386775598149 19.7131224064077699   T   T   T
  1.4527291747752304  5.1432059967551780 21.9266485315414883   T   T   T
  3.7951762262661708  3.8021939508160254 21.9363164125885213   T   T   T
  2.2402133725833946  3.8213693092668786 24.0805565713404732   T   T   T
  3.0226045799548924  5.1670069016391427 19.8183733428637190   T   T   T
  4.5487063135006345  5.1540316664868504 24.0925559048743416   T   T   T
  5.3568221275283712  1.1290821711084786 19.8170792046460669   T   T   T
  6.1284664986566195  2.4934434194672979 21.8997547699862345   T   T   T
  8.4096427688032289  1.1741927072601301 21.9307177557616413   T   T   T
  6.8694794738002489  1.1393760726695878 24.0778886548730426   T   T   T
  7.6632790545646277  2.5291352761480899 19.6370435075089134   T   T   T
  9.1988922579257473  2.4733166810724838 24.0866963172986246   T   T   T
  5.2913340272583378  3.7713430871905862 19.6939831259864633   T   T   T
  6.0908105020209193  5.1294522838287051 21.9264530091414365   T   T   T
  8.4425923105126355  3.8049475238187158 21.9006447417861771   T   T   T
  6.8786868068198705  3.8174397014146479 24.0783043435165141   T   T   T
  7.6537549192618677  5.1891674216718267 19.8898584655725230   T   T   T
  9.1780263311162660  5.1491454984257103 24.0719156267592282   T   T   T

Oxide reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Rh E_tot= -214.53322517 eV
 D3-zero damping= -7.9951445 eV, D3-BJ damping= -8.8893886 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     9.2756956675135616    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3553253905600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.3092812387561530
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2
Selective dynamics
Cartesian
  3.0918226213437685  5.3503169460745283  8.9451241821253618   F   F   F
  1.5458752422699680  2.6726542696091213  8.0000001838787966   F   F   F
  3.0918231281762156  3.3199547705521724  8.9451248436730744   F   F   F
  1.5458743861009421  0.6422920909319076  8.0000000000000000   F   F   F
  1.5458776778471819  5.3503168726290991 11.7805090714841079   F   F   F
  3.0918288546112342  2.6726541961636912 10.8353850732375427   F   F   F
  1.5458781846796272  3.3199546971067431 11.7805097330318205   F   F   F
  3.0918279984422088  0.6422920174864777 10.8353848893587461   F   F   F
  3.0917662050067194  5.2888542817311182 14.6436780696748023   T   T   T
  1.5458253880054615  2.6491946903968366 13.6917512867603275   T   T   T
  3.0917869687269577  3.3110175232009351 14.7370350355613144   T   T   T
  1.5458396166505122  0.6554030923517520 13.6645444257965600   T   T   T
  1.5459316276539132  5.0676756763532760 17.2736306875020915   T   T   T
  3.0917782002327403  2.6101351354467579 16.6935706381790858   T   T   T
  1.5458490054207530  3.2582227339414409 17.6582618051658962   T   T   T
  3.0918385787340661  0.6315179353519215 16.5559821444269240   T   T   T
  6.1837211771816225  5.3503169460745283  8.9451241821253618   F   F   F
  4.6377737981078218  2.6726542696091213  8.0000001838787966   F   F   F
```

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  6.1837216840140687  3.3199547705521724  8.9451248436730744   F   F   F
  4.6377729419387963  0.6422920909319076  8.0000000000000000   F   F   F
  4.6377762336850354  5.3503168726290991 11.7805090714841079   F   F   F
  6.1837274104490891  2.6726541961636912 10.8353850732375427   F   F   F
  4.6377767405174808  3.3199546971067431 11.7805097330318205   F   F   F
  6.1837265542800628  0.6422920174864777 10.8353848893587461   F   F   F
  6.1836641267990142  5.2888529154848953 14.6436523055669614   T   T   T
  4.6377207254496691  2.6491937633048375 13.6917362328744758   T   T   T
  6.1836900174732481  3.3110178411218891 14.7370321302940361   T   T   T
  4.6377269284520803  0.6554100976281628 13.6645460974231661   T   T   T
  4.6378186935984758  5.0676626061454817 17.2735780990325551   T   T   T
  6.1836902635057784  2.6101396601353395 16.6935749227340331   T   T   T
  4.6377479571004434  3.2582393337166979 17.6582426433399107   T   T   T
  6.1837534465357038  0.6315248666811190 16.5559612127279117   T   T   T
  9.2756197330194770  5.3503169460745283  8.9451241821253618   F   F   F
  7.7296723539456753  2.6726542696091213  8.0000001838787966   F   F   F
  9.2756202398519214  3.3199547705521724  8.9451248436730744   F   F   F
  7.7296714977766490  0.6422920909319076  8.0000000000000000   F   F   F
  7.7296747895228908  5.3503168726290991 11.7805090714841079   F   F   F
  9.2756259662869436  2.6726541961636912 10.8353850732375427   F   F   F
  7.7296752963553352  3.3199546971067431 11.7805097330318205   F   F   F
  9.2756251101179163  0.6422920174864777 10.8353848893587461   F   F   F
 -0.0001250735277248  5.2888412008827288 14.6436592145609321   T   T   T
  7.7296198626051122  2.6491877212385795 13.6917302627488660   T   T   T
  9.2755919562383884  3.3110065915423417 14.7370263221111557   T   T   T
  7.7296372871983587  0.6554057187946171 13.6645430975684441   T   T   T
  7.7297161769332074  5.0676537285927274 17.2735871173180833   T   T   T
  9.2755905412550241  2.6101262472687141 16.6935533525386219   T   T   T
  7.7296627018850499  3.2582310070014948 17.6582456126884644   T   T   T
  9.2756557149329897  0.6315101358960266 16.5559634790464685   T   T   T

Metal reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Rh E_tot= -170.59248435 eV
 D3-zero damping= -8.6650034 eV, D3-BJ damping= -10.4569284 eV
Rh
 1.0000000000000000
     9.2756956675135616    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3553253905600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.5552264120280803
  24
Cartesian
  0.5300566962355565  0.9094021724479541  8.1318877374619216
  1.2964270225722097  2.2494254097946844 10.2775415271634305
  3.6154289455688309  0.9106887099374533 10.2777037458500722
  2.0654604933705119  0.9091312562298607 12.4231812875426950
  2.8490808866618682  2.2482229471804738  8.1320318507101064
  4.3842415510742399  2.2480347588407530 12.4233086867429350
  0.5300173708883182  3.5870090415816436  8.1318686492107517
  1.2964201450226525  4.9270933758386342 10.2775281572434061
  3.6154340464670405  3.5883224786059627 10.2777589968207508
  2.0655299480217111  3.5868286016957138 12.4232295198437885
  2.8489773980640321  4.9258436454183308  8.1320511916322697
  4.3843318556570319  4.9256193709025338 12.4233293620504526
  5.1678462051476020  0.9093562005225494  8.1319334782428641
  5.9342364535974381  2.2493719432446087 10.2777133475756237
  8.2531378550666670  0.9104864653623115 10.2776133248114405
  6.7033331292993488  0.9090920920296937 12.4232151082729239
  7.4868389775551245  2.2481773055915273  8.1318798364467444
  9.0223018067187599  2.2479418946459160 12.4231502433409116
  5.1678230301884742  3.5869966596210410  8.1318997444081287
  5.9342750489274829  4.9268875880716250 10.2776519128346902
  8.2532323832288714  3.5880567835979260 10.2775910609943431
  6.7033902018830922  3.5868336244801813 12.4232373762245274
  7.4868678449707469  4.9258525439860428  8.1319028900995960
```

```
  9.0221500217414583  4.9254470956968648 12.4231181180182784

Interface: ZnO(10-10)/fcc(111)_2sqrt3x2/Os E_tot= -480.01177237 eV
 D3-zero damping= -19.399867 eV, D3-BJ damping= -21.7235488 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Os
 1.0000000000000000
     9.3822222924795931    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4168285661600013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.1021996581789182
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2  24
Selective dynamics
Cartesian
  3.1273306242635828  5.4117626022488725  8.9451241821253618   F   F   F
  1.5636288295027094  2.7033483381995405  8.0000001838787966   F   F   F
  3.1273311369167409  3.3580827546327026  8.9451248436730744   F   F   F
  1.5636279635010197  0.6496684873922814  8.0000000000000000   F   F   F
  1.5636312930512830  5.4117625279599588 11.7805090714841079   F   F   F
  3.1273369291169399  2.7033482639106272 10.8353850732375427   F   F   F
  1.5636318057044403  3.3580826803437898 11.7805097330318205   F   F   F
  3.1273360631152509  0.6496684131033682 10.8353848893587461   F   F   F
  3.1323788440821585  5.4080851116776882 14.6780825031752240   T   T   T
  1.5974415341084736  2.6828608979634452 13.6879158547974029   T   T   T
  3.1305252093903739  3.4074062018040352 14.7692013778894342   T   T   T
  1.5866235099662309  0.6858840617724025 13.6493879607304311   T   T   T
  1.5926129942076113  5.5632624137020636 17.5645222606483635   T   T   T
  3.1335010848826039  2.7990640307593404 16.7121833093604941   T   T   T
  1.4628044253255461  3.5364816716095921 17.5803218455268180   T   T   T
  3.1414629238032452  0.8026567557605974 16.4899116305486650   T   T   T
  6.2547380550901135  5.4117626022488725  8.9451241821253618   F   F   F
  4.6910362603292404  2.7033483381995405  8.0000001838787966   F   F   F
  6.2547385677432716  3.3580827546327026  8.9451248436730744   F   F   F
  4.6910353943275505  0.6496684873922814  8.0000000000000000   F   F   F
  4.6910387238778135  5.4117625279599588 11.7805090714841079   F   F   F
  6.2547443599434711  2.7033482639106272 10.8353850732375427   F   F   F
  4.6910392365309708  3.3580826803437898 11.7805097330318205   F   F   F
  6.2547434939417821  0.6496684131033682 10.8353848893587461   F   F   F
  6.2343243210723189  5.3481804412446179 14.5966503024240435   T   T   T
  4.6618508760742490  2.6825101362104471 13.6874550571394078   T   T   T
  6.2609279879449815  3.3565513983948843 14.6778889759697915   T   T   T
  4.6783033085371084  0.6852485009974725 13.6491597922491863   T   T   T
  4.6825543964925727  5.5401430235471603 17.5613286766004499   T   T   T
  6.2515864148946729  2.6350589020867674 16.5427899531252081   T   T   T
  4.8120611510776232  3.5047407373321091 17.5907937918629997   T   T   T
  6.2461775919832609  0.6504184558948950 16.4467145075909826   T   T   T
  9.3821454859166451  5.4117626022488725  8.9451241821253618   F   F   F
  7.8184436911557702  2.7033483381995405  8.0000001838787966   F   F   F
  9.3821459985698006  3.3580827546327026  8.9451248436730744   F   F   F
  7.8184428251540803  0.6496684873922814  8.0000000000000000   F   F   F
  7.8184461547043451  5.4117625279599588 11.7805090714841079   F   F   F
  9.3821517907700027  2.7033482639106272 10.8353850732375427   F   F   F
  7.8184466673575015  3.3580826803437898 11.7805097330318205   F   F   F
  9.3821509247683128  0.6496684131033682 10.8353848893587461   F   F   F
  0.0301336373890877  5.3515239108516761 14.5978901984087663   T   T   T
  7.8220923202540265  2.6482352114288630 13.6557749849584891   T   T   T
  9.3815726895448801  3.3606275139456132 14.6772587979706781   T   T   T
  7.8228486065913136  0.6541216430126388 13.6582873840135992   T   T   T
  7.8338921873785212  5.2994901408267268 17.3327150620865851   T   T   T
  9.4051425145450107  2.6486394927637802 16.5473413438935886   T   T   T
  7.8236191091238085  3.2499810780943710 17.5943585512532650   T   T   T
  9.4121710002527390  0.6650858068588114 16.4436805364257950   T   T   T
  0.7658481714274687  1.2847084955643657 19.8348835176087697   T   T   T
  1.5785527268594051  2.6588670862485175 21.9497748475552292   T   T   T
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  3.9305243814585826  1.3057621850850936 21.9560562462583206   T   T   T
  2.3627595028625712  1.3049197441233475 24.1044087475595106   T   T   T
  3.1410089148342437  2.6533966647096090 19.8533507432257892   T   T   T
  4.7015407461717222  2.6623876379553910 24.0992459134429957   T   T   T
  0.8576527246683260  3.9469441608956872 19.7686799356039380   T   T   T
  1.5556643246154347  5.3622698525232986 21.9520410703116333   T   T   T
  3.9329132633648087  4.0049118845292471 21.9584090830468313   T   T   T
  2.3566661065287251  4.0009689308651133 24.1050178072614720   T   T   T
  3.1432869752206947  5.4158947580458205 19.8235341303901080   T   T   T
  4.7036026815227769  5.3551646385219831 24.1058691737774531   T   T   T
  5.5157783420938982  1.2703879307911297 19.8306264215699741   T   T   T
  6.2893977219996362  2.6768635780964369 21.9419508448228946   T   T   T
  8.5968993833611638  1.3191007565410913 21.9811591838202105   T   T   T
  7.0498515575712393  1.3090645692355902 24.1010815584463423   T   T   T
  7.8417232324991684  2.7127989090283648 19.7151147633120409   T   T   T
  9.3926035860300630  2.6647850586482953 24.1125602064512954   T   T   T
  5.4275837984202644  3.9494569156411887 19.7668648139319103   T   T   T
  6.2556955272295456  5.3468524238175306 21.9541323304780533   T   T   T
  8.6300267256168350  3.9900617482664691 21.9257003404969240   T   T   T
  7.0465812741132172  4.0000542993090287 24.1002535656707195   T   T   T
  7.8374165185370037  5.4027479182419640 19.8719847634621445   T   T   T
  9.3987336149910217  5.3521708142510507 24.0980168085937372   T   T   T

Oxide reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Os E_tot= -214.87315005 eV
 D3-zero damping= -7.9043437 eV, D3-BJ damping= -8.7341654 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     9.3822222924795931    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4168285661600013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.3092812387561530
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2
Selective dynamics
Cartesian
  3.1273306242635828  5.4117626022488725  8.9451241821253618   F   F   F
  1.5636288295027094  2.7033483381995405  8.0000001838787966   F   F   F
  3.1273311369167409  3.3580827546327026  8.9451248436730744   F   F   F
  1.5636279635010197  0.6496684873922814  8.0000000000000000   F   F   F
  1.5636312930512830  5.4117625279599588 11.7805090714841079   F   F   F
  3.1273369291169399  2.7033482639106272 10.8353850732375427   F   F   F
  1.5636318057044403  3.3580826803437898 11.7805097330318205   F   F   F
  3.1273360631152509  0.6496684131033682 10.8353848893587461   F   F   F
  3.1272416877135432  5.3382488351665387 14.6048957909567267   T   T   T
  1.5636093607510528  2.6702620528621299 13.6843378981110035   T   T   T
  3.1273158905741787  3.3537386943616805 14.6946763093806645   T   T   T
  1.5635568417625987  0.6665116594341772 13.6627997144337279   T   T   T
  1.5636763307917916  5.1218800291888575 17.1933466027761064   T   T   T
  3.1273622309834264  2.6291131418832072 16.6563470278215107   T   T   T
  1.5636556094510117  3.3074493235903333 17.5687963780857430   T   T   T
  3.1273874055009294  0.6403434248617611 16.5251700299262225   T   T   T
  6.2547380550901135  5.4117626022488725  8.9451241821253618   F   F   F
  4.6910362603292404  2.7033483381995405  8.0000001838787966   F   F   F
  6.2547385677432716  3.3580827546327026  8.9451248436730744   F   F   F
  4.6910353943275505  0.6496684873922814  8.0000000000000000   F   F   F
  4.6910387238778135  5.4117625279599588 11.7805090714841079   F   F   F
  6.2547443599434711  2.7033482639106272 10.8353850732375427   F   F   F
  4.6910392365309708  3.3580826803437898 11.7805097330318205   F   F   F
  6.2547434939417821  0.6496684131033682 10.8353848893587461   F   F   F
  6.2546451680636928  5.3382440062743841 14.6049082307453748   T   T   T
  4.6910166607402646  2.6702605123933076 13.6843364579127442   T   T   T
  6.2547230646395429  3.3537334108495584 14.6946786866609358   T   T   T
  4.6909694949054819  0.6665112694692436 13.6627986267630526   T   T   T
  4.6910833087593744  5.1218787371234642 17.1933882955358079   T   T   T
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  6.2547725950727315  2.6291077817632109 16.6563463175047879   T   T   T
  4.6910702276453806  3.3074433380120802 17.5688089699729311   T   T   T
  6.2547870097637279  0.6403380766547956 16.5251769738465448   T   T   T
  9.3821454859166451  5.4117626022488725  8.9451241821253618   F   F   F
  7.8184436911557702  2.7033483381995405  8.0000001838787966   F   F   F
  9.3821459985698006  3.3580827546327026  8.9451248436730744   F   F   F
  7.8184428251540803  0.6496684873922814  8.0000000000000000   F   F   F
  7.8184461547043451  5.4117625279599588 11.7805090714841079   F   F   F
  9.3821517907700027  2.7033482639106272 10.8353850732375427   F   F   F
  7.8184466673575015  3.3580826803437898 11.7805097330318205   F   F   F
  9.3821509247683128  0.6496684131033682 10.8353848893587461   F   F   F
 -0.0001739342709016  5.3382439142558500 14.6048942087180205   T   T   T
  7.8184209486926743  2.6702586277738400 13.6843321625298291   T   T   T
  9.3821261123079669  3.3537357755644948 14.6946733246464998   T   T   T
  7.8183689338905085  0.6665106239165154 13.6627972218361204   T   T   T
  7.8184914336399203  5.1218806776421895 17.1933873780856885   T   T   T
  9.3821682945310023  2.6291119090072517 16.6563409586395750   T   T   T
  7.8184735267666383  3.3074462382295913 17.5688157637059028   T   T   T
  9.3821877767568083  0.6403424191349383 16.5251659895162852   T   T   T

Metal reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Os E_tot= -258.94900154 eV
 D3-zero damping= -8.5771576 eV, D3-BJ damping= -10.1040612 eV
Os
 1.0000000000000000
     9.3822222924795931    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4168285661600013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.5552264120280803
  24
Cartesian
  0.5382548080117202  0.9201623587274754  8.1339890509027004
  1.3121454821330785  2.2746393011824821 10.2774057580640381
  3.6576601207634591  0.9203215763144329 10.2777445620506693
  2.0862721103505151  0.9199925403986452 12.4211864860209023
  2.8837387503070064  2.2742472835009262  8.1340163328345554
  4.4317457342532229  2.2742119025662015 12.4212879982290829
  0.5382558901120350  3.6285324040710836  8.1339653292463439
  1.3121461141356172  4.9830955325094992 10.2774435441881522
  3.6576758329402943  3.6286734235331273 10.2776290133955719
  2.0862950172489327  3.6283807150091607 12.4211932189689094
  2.8838517274018245  4.9827141768591492  8.1340063317654838
  4.4317379872729967  4.9826157249015557 12.4212904852565416
  5.2293265431283418  0.9199464318813458  8.1339536811145763
  6.0033245732827769  2.2744952077603435 10.2776053894680679
  8.3488587001027437  0.9203981693903357 10.2776174812142358
  6.7773832327470194  0.9199773723400300 12.4211776806511640
  7.5748883425570224  2.2741435939249652  8.1339543987622438
  9.1228893202360126  2.2742120154320693 12.4212232805379976
  5.2293201354291350  3.6283641864913738  8.1339477798067410
  6.0033427909994828  4.9829512096732573 10.2776152327885217
  8.3488738094169008  3.6287428044122398 10.2776733938122415
  6.7773939384251802  3.6283901753001349 12.4211822877027629
  7.5748924073186990  4.9825328959158162  8.1339542612345017
  9.1228818236710190  4.9826418216345436 12.4212640794974991

Interface: ZnO(10-10)/fcc(111)_2sqrt3x2/Ru E_tot= -435.36938481 eV
 D3-zero damping= -20.1998499 eV, D3-BJ damping= -21.8320799 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Ru
 1.0000000000000000
     9.2359695118261431    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3323894838800010    0.0000000000000000
     0.0000000000000000    0.0000000000000000   32.1021996581789182
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2  24
```

Selective dynamics
Cartesian

3.0785808946619024	5.3274024896719538	8.9451241821253618	F	F	F
1.5392545334035885	2.6612077664659672	8.0000001838787966	F	F	F
3.0785813993236757	3.3057359944282361	8.9451248436730744	F	F	F
1.5392536809013824	0.6395412680809034	8.0000000000000000	F	F	F
1.5392569585496583	5.3274024165410783	11.7805090714841079	F	F	F
3.0785871012333916	2.6612076933350908	10.8353850732375427	F	F	F
1.5392574632114304	3.3057359212973605	11.7805097330318205	F	F	F
3.0785862487311859	0.6395411949500270	10.8353848893587461	F	F	F
3.0755313560563731	5.3179842089518612	14.6991279777141610	T	T	T
1.5502340110943942	2.6508874648290646	13.6932617549251887	T	T	T
3.0741380330661197	3.3296928971252675	14.7913664892357328	T	T	T
1.5481300637699738	0.6665764894126719	13.6511857495824103	T	T	T
1.5556202117508802	5.4381722814618545	17.6481031773389141	T	T	T
3.0607756760395470	2.7049221525898499	16.7092805698830489	T	T	T
1.4711717520434864	3.4079336676218177	17.6957868760870447	T	T	T
3.0719010530886162	0.7241588170612803	16.5277816048185358	T	T	T
6.1572373986039501	5.3274024896719538	8.9451241821253618	F	F	F
4.6179110373456362	2.6612077664659672	8.0000001838787966	F	F	F
6.1572379032657230	3.3057359944282361	8.9451248436730744	F	F	F
4.6179101848434296	0.6395412680809034	8.0000000000000000	F	F	F
4.6179134624917060	5.3274024165410783	11.7805090714841079	F	F	F
6.1572436051754398	2.6612076933350908	10.8353850732375427	F	F	F
4.6179139671534779	3.3057359212973605	11.7805097330318205	F	F	F
6.1572427526732332	0.6395411949500270	10.8353848893587461	F	F	F
6.1382303855693525	5.2829904413943192	14.6665424928193904	T	T	T
4.5984525841720219	2.6473538571154838	13.6922305570319658	T	T	T
6.1563979892372220	3.2987302227309621	14.7423653340624217	T	T	T
4.6069448808332432	0.6619405116044018	13.6545003206624997	T	T	T
4.5732422471427965	5.3892435369272329	17.6396397036252424	T	T	T
6.1378836519301387	2.6150686976032880	16.6252291287166472	T	T	T
4.6654018198458820	3.3686743265233225	17.6779282783048650	T	T	T
6.1202347103549144	0.6371645174718019	16.5223435728064274	T	T	T
9.2358939025459978	5.3274024896719538	8.9451241821253618	F	F	F
7.6965675412876831	2.6612077664659672	8.0000001838787966	F	F	F
9.2358944072077680	3.3057359944282361	8.9451248436730744	F	F	F
7.6965666887854765	0.6395412680809034	8.0000000000000000	F	F	F
7.6965699664337537	5.3274024165410783	11.7805090714841079	F	F	F
9.2359001091174875	2.6612076933350908	10.8353850732375427	F	F	F
7.6965704710955256	3.3057359212973605	11.7805097330318205	F	F	F
9.2358992566152800	0.6395411949500270	10.8353848893587461	F	F	F
0.0157950529336611	5.2913288945340176	14.6597953050432981	T	T	T
7.6957793903837217	2.6298821951430802	13.6775286699446390	T	T	T
9.2302444113247812	3.3081898429818399	14.7472863934449485	T	T	T
7.6921102604409590	0.6444405405948770	13.6643243278588464	T	T	T
7.7040156322573106	5.3278678351486395	17.4925121007956221	T	T	T
9.2296418297096441	2.6428585022311171	16.6385918295337056	T	T	T
7.6703060604319449	3.2717493753180227	17.6954946298378530	T	T	T
9.2618200615117487	0.6653211460920636	16.5068965689687168	T	T	T
0.6301389068400428	1.1112018597718867	19.8727427676953070	T	T	T
1.4544437264324686	2.4377444585140053	21.9450856990767953	T	T	T
3.7650269556285099	1.1070663183376095	21.9374605978048400	T	T	T
2.2225948417099453	1.0952991025315779	24.0703703923925723	T	T	T
2.9823406810382469	2.4173816363354885	19.8543489270448106	T	T	T
4.5260062553805884	2.4264940912514361	24.0702543002781759	T	T	T
0.7353914302166492	3.7215942589401312	19.8008422529001038	T	T	T
1.4345962583759870	5.1002745724176561	21.9477829903539892	T	T	T
3.7699711121128736	3.7546113920440947	21.9596194713383248	T	T	T
2.2108658884807495	3.7508998235612006	24.0712368563300849	T	T	T
3.0058467589933118	5.1292010986435930	19.8807768529357851	T	T	T
4.5240216238908406	5.0747014943980613	24.0824041770862465	T	T	T
5.3439131638281356	1.1042721637034003	19.8804825181890941	T	T	T

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  6.0868480009686268  2.4603645992829906 21.9651792253178790   T   T   T
  8.3537064841930810  1.1060078624610663 21.9776601596136736   T   T   T
  6.8359185434940750  1.1081368519718404 24.0830580223206034   T   T   T
  7.6338813485979511  2.4871579205286198 19.7317991501700050   T   T   T
  9.1490138748762906  2.4288163976678421 24.0924801521821621   T   T   T
  5.2472160478560435  3.7200506297789495 19.7971217425944843   T   T   T
  6.0506690771658569  5.0854029101441025 21.9631675667899842   T   T   T
  8.3983556978391363  3.7387839680655688 21.9528838493814575   T   T   T
  6.8295020032901768  3.7477788424361411 24.0844313191813733   T   T   T
  7.6097129188675758  5.0993432084024350 19.9480549510396301   T   T   T
  9.1504715030477293  5.0698242876788049 24.0735480695135635   T   T   T

Oxide reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Ru E_tot= -214.32777838 eV
 D3-zero damping= -8.0322501 eV, D3-BJ damping= -8.9496726 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     9.2359695118261431    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3323894838800010    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.3092812387561530
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2
Selective dynamics
Cartesian
  3.0785808946619024  5.3274024896719538  8.9451241821253618   F   F   F
  1.5392545334035885  2.6612077664659672  8.0000001838787966   F   F   F
  3.0785813993236757  3.3057359944282361  8.9451248436730744   F   F   F
  1.5392536809013824  0.6395412680809034  8.0000000000000000   F   F   F
  1.5392569585496583  5.3274024165410783 11.7805090714841079   F   F   F
  3.0785871012333916  2.6612076933350908 10.8353850732375427   F   F   F
  1.5392574632114304  3.3057359212973605 11.7805097330318205   F   F   F
  3.0785862487311859  0.6395411949500270 10.8353848893587461   F   F   F
  3.0786224694199915  5.2752718002299499 14.6576997435069263   T   T   T
  1.5393072487705617  2.6445231028094982 13.6927510833771002   T   T   T
  3.0786382617451511  3.2977909497410285 14.7503219115539022   T   T   T
  1.5393231218047079  0.6535092586498219 13.6640153132195632   T   T   T
  1.5392392459176016  5.0489022193350879 17.3040179950749611   T   T   T
  3.0786199679084070  2.6041968688980295 16.7049149721343078   T   T   T
  1.5392717637731790  3.2402190768431529 17.6886909755993535   T   T   T
  3.0785821988768323  0.6298776772100148 16.5683754615415708   T   T   T
  6.1572373986039501  5.3274024896719538  8.9451241821253618   F   F   F
  4.6179110373456362  2.6612077664659672  8.0000001838787966   F   F   F
  6.1572379032657230  3.3057359944282361  8.9451248436730744   F   F   F
  4.6179101848434296  0.6395412680809034  8.0000000000000000   F   F   F
  4.6179134624917060  5.3274024165410783 11.7805090714841079   F   F   F
  6.1572436051754398  2.6612076933350908 10.8353850732375427   F   F   F
  4.6179139671534779  3.3057359212973605 11.7805097330318205   F   F   F
  6.1572427526732332  0.6395411949500270 10.8353848893587461   F   F   F
  6.1572766587617620  5.2752563911767227 14.6576907760225854   T   T   T
  4.6179502613419787  2.6445662214242813 13.6927764847731623   T   T   T
  6.1572820565256823  3.2977744104112254 14.7503105609818927   T   T   T
  4.6179745770998100  0.6535007566416668 13.6640135937244374   T   T   T
  4.6178933030701224  5.0488945722124043 17.3040211105187325   T   T   T
  6.1572684498711521  2.6041882699140801 16.7049150024007993   T   T   T
  4.6179272220579062  3.2402137529071231 17.6887028970512326   T   T   T
  6.1572340468922073  0.6298692147802953 16.5683696799649951   T   T   T
  9.2358939025459978  5.3274024896719538  8.9451241821253618   F   F   F
  7.6965675412876831  2.6612077664659672  8.0000001838787966   F   F   F
  9.2358944072077680  3.3057359944282361  8.9451248436730744   F   F   F
  7.6965666887854765  0.6395412680809034  8.0000000000000000   F   F   F
  7.6965699664337537  5.3274024165410783 11.7805090714841079   F   F   F
  9.2359001091174875  2.6612076933350908 10.8353850732375427   F   F   F
  7.6965704710955256  3.3057359212973605 11.7805097330318205   F   F   F
  9.2358992566152800  0.6395411949500270 10.8353848893587461   F   F   F
```

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 -0.0000312412311058  5.2752697635963441 14.6576927422425740   T   T   T
  7.6966201359271977  2.6445349972258376 13.6927684215628140   T   T   T
  9.2359568618107009  3.2977879546351563 14.7503201438944060   T   T   T
  7.6966329997161393  0.6535061551350664 13.6640172110993596   T   T   T
  7.6965507122317733  5.0488912898572300 17.3040070850908272   T   T   T
  9.2359301083399643  2.6041924770266207 16.7049194218715158   T   T   T
  7.6965804417468453  3.2402117208832872 17.6886946136344037   T   T   T
  9.2358927370329393  0.6298747646679508 16.5683718437374594   T   T   T

Metal reference: ZnO(10-10)/fcc(111)_2sqrt3x2/Ru E_tot= -213.787533 eV
 D3-zero damping= -8.282346 eV, D3-BJ damping= -10.0632461 eV
Ru
 1.0000000000000000
     9.2359695118261431    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3323894838800010    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.5552264120280803
  24
Cartesian
  0.5256306782737226  0.9057848619783025  8.1671367558388095
  1.2900409723985147  2.2392106419247821 10.2775806670662213
  3.5989936293578064  0.9060463341953887 10.2773635690768987
  2.0596733108995902  0.9056015336494506 12.3880785876375992
  2.8344648096765814  2.2387798031723878  8.1666054063635194
  4.3684645853584456  2.2386156073127452 12.3880438213750423
  0.5255925599243491  3.5720184045193966  8.1672199913344947
  1.2900690751845061  4.9052319378049853 10.2776268667965667
  3.5990303689268521  3.5722180980125828 10.2774288130083278
  2.0596892153301893  3.5719134200270108 12.3879461922027811
  2.8347439857815848  4.9049571964122878  8.1667122934690486
  4.3686239373298710  4.9046058322512289 12.3878711655596963
  5.1439636277386498  0.9058773469751051  8.1669469693201986
  5.9079868181865978  2.2392989412692033 10.2775839299827680
  8.2168110389391753  0.9060720905848679 10.2778622210444741
  6.6775499538505789  0.9055379376572317 12.3883708260151710
  7.4524901799694296  2.2387531762568522  8.1672603023561479
  8.9867587422449464  2.2384091399443817 12.3883422941278045
  5.1437684432655084  3.5720005914326665  8.1670079355152243
  5.9078072020672359  4.9053023729427441 10.2777270697433707
  8.2167725511306209  3.5724522925070219 10.2779394574279674
  6.6775761343462330  3.5718912808316188 12.3883159410101520
  7.4528183534449992  4.9050594878584466  8.1670866592706179
  8.9866360136588135  4.9045568328275264 12.3882695568028804

Interface: TiO2(110)/fcc(111)_7x3sqrt3/Au E_tot= -3637.89727394 eV
 D3-zero damping= -124.911456517 eV, D3-BJ damping= -140.750472695 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Au
 1.0000000000000000
    20.2912619732900055    0.0000000000000012    0.0000000000000000
     0.0000000000000009   15.0623557231836873    0.0000000000000000
     0.0000000000000000    0.0000000000000000   35.3289349005892035
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4
2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2
4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4
2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2
```

```
4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2
2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2 126
Selective dynamics
Cartesian
  0.0000000000000007  1.5062355723183694  9.2861208469999976   F   F   F
  0.0000000000000005  0.0000000000000005  7.9999999999999982   F   F   F
  2.0578045142512513  1.5062355723183694  9.2861208469999976   F   F   F
  3.3818769955483345  0.0000000000000006  9.2861208469999976   F   F   F
  3.3818769955483345  1.5062355723183696 12.5708101129999950   F   F   F
  3.3818769955483345  0.0000000000000007 11.2846892659999956   F   F   F
  0.0000000000000007  0.0000000000000007 10.5722416939999970   F   F   F
  4.7059494768454186  1.5062355723183694  9.2861208469999976   F   F   F
  5.4396815097995859  1.5062355723183696 12.5708101129999950   F   F   F
  0.0000000000000008  0.0000000000000008 12.5708101129999950   F   F   F
 20.0467859076869779  1.5074426765967566 15.8126334752017481   T   T   T
 -0.0078697858911096  0.0026541900972651 14.6246110235074394   T   T   T
  3.3818769955483345  0.0000000000000009 13.8569309599999944   F   F   F
  1.3240724812970845  1.5062355723183696 12.5708101129999950   F   F   F
  2.1057188029333385  1.5020532819893071 15.8470984662602543   T   T   T
  3.3610965438375744  0.0680219893219232 15.8782368414403905   T   T   T
  3.2195790806055213  1.5054855728262333 19.1447032237867987   T   T   T
  3.3721894966261821 -0.0146894982809583 17.8007849948344692   T   T   T
 20.2646501148425635  0.0002747855258220 17.1639185008065986   T   T   T
  4.7300974554644810  1.4908481237462141 15.8458789466154641   T   T   T
  5.5004164770976773  1.5058182512962175 19.2368830184145878   T   T   T
 -0.0669797368107178  0.0061855257565191 19.0228706096438529   T   T   T
  3.3805222332385805  0.0303889232202875 20.3196053790753837   T   T   T
  1.2772957991424700  1.4951907025259374 19.2209924022598422   T   T   T
  0.0000000000000009  4.5187067169551076  9.2861208469999976   F   F   F
  0.0000000000000007  3.0124711446367378  7.9999999999999982   F   F   F
  2.0578045142512513  4.5187067169551076  9.2861208469999976   F   F   F
  3.3818769955483345  3.0124711446367378  9.2861208469999976   F   F   F
  3.3818769955483345  4.5187067169551076 12.5708101129999950   F   F   F
  3.3818769955483345  3.0124711446367383 11.2846892659999956   F   F   F
  0.0000000000000009  3.0124711446367378 10.5722416939999970   F   F   F
  4.7059494768454186  4.5187067169551076  9.2861208469999976   F   F   F
  5.4396815097995859  4.5187067169551076 12.5708101129999950   F   F   F
  0.0000000000000010  3.0124711446367383 12.5708101129999950   F   F   F
 20.0730849323006453  4.5110134346359034 15.8089566988653356   T   T   T
 -0.0268306899262335  3.0072794564243779 14.6224364103773681   T   T   T
  3.3818769955483345  3.0124711446367383 13.8569309599999944   F   F   F
  1.3240724812970848  4.5187067169551076 12.5708101129999950   F   F   F
  2.0675303823299691  4.5321118627106296 15.8479207335587020   T   T   T
  3.2438984275845471  3.0409452044927332 15.8731945994294836   T   T   T
  3.3569875606812349  4.5249067183151697 19.1410213013704080   T   T   T
  3.3763176900041079  3.0135446860133874 17.7952909246809767   T   T   T
 20.2463032074005689  3.0105347111143206 17.1644142716045600   T   T   T
  4.7080733516985216  4.5161680049372217 15.8410195033472032   T   T   T
  5.4908986755650524  4.5236678850890648 19.2320724677859012   T   T   T
 -0.1003702816105662  3.0332864807120532 19.0424723137028948   T   T   T
  3.3792283497733391  3.0141848684934183 20.2895789415018371   T   T   T
  1.2943238458390516  4.5236593257832292 19.2095681644427572   T   T   T
  0.0000000000000011  7.5311778615918454  9.2861208469999976   F   F   F
  0.0000000000000009  6.0249422892734756  7.9999999999999982   F   F   F
  2.0578045142512518  7.5311778615918454  9.2861208469999976   F   F   F
  3.3818769955483350  6.0249422892734756  9.2861208469999976   F   F   F
  3.3818769955483350  7.5311778615918454 12.5708101129999950   F   F   F
  3.3818769955483350  6.0249422892734756 11.2846892659999956   F   F   F
  0.0000000000000010  6.0249422892734756 10.5722416939999970   F   F   F
  4.7059494768454186  7.5311778615918454  9.2861208469999976   F   F   F
  5.4396815097995859  7.5311778615918454 12.5708101129999950   F   F   F
  0.0000000000000012  6.0249422892734756 12.5708101129999950   F   F   F
 20.1449358657785638  7.5325054582290107 15.7993282549036049   T   T   T
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-0.0148191821128099	6.0315007195915449	14.6213567905855939	T	T	T
3.3818769955483350	6.0249422892734756	13.8569309599999944	F	F	F
1.3240724812970850	7.5311778615918454	12.5708101129999950	F	F	F
2.0625605383863346	7.5436511675829347	15.8546326303376066	T	T	T
3.2390136789948474	6.0611405720293901	15.8710552751745588	T	T	T
3.5250147779975585	7.5261945488124002	19.1664688287942155	T	T	T
3.3893661314077215	6.0337808871408676	17.8024333449560714	T	T	T
20.2816512310655561	6.0320273235515653	17.1620474588780141	T	T	T
4.7155959921764570	7.5256141573405673	15.8495968560290912	T	T	T
5.4843509117369083	7.5203955334299009	19.2545988870771332	T	T	T
0.0683545339266311	6.0126312848159191	19.0168496549597634	T	T	T
3.3919047183548061	5.9993951751402514	20.3254678578030941	T	T	T
1.2784196979184843	7.5308275285295174	19.2431357705512731	T	T	T
0.0000000000000012	10.5436490062285841	9.2861208469999976	F	F	F
0.0000000000000011	9.0374134339102152	7.9999999999999982	F	F	F
2.0578045142512518	10.5436490062285841	9.2861208469999976	F	F	F
3.3818769955483350	9.0374134339102152	9.2861208469999976	F	F	F
3.3818769955483350	10.5436490062285841	12.5708101129999950	F	F	F
3.3818769955483350	9.0374134339102152	11.2846892659999956	F	F	F
0.0000000000000012	9.0374134339102152	10.5722416939999970	F	F	F
4.7059494768454195	10.5436490062285841	9.2861208469999976	F	F	F
5.4396815097995868	10.5436490062285841	12.5708101129999950	F	F	F
0.0000000000000014	9.0374134339102152	12.5708101129999950	F	F	F
20.1252695119836176	10.5560160546414696	15.8076843216080150	T	T	T
0.0003956070784834	9.0507626561248529	14.6252632081485494	T	T	T
3.3818769955483350	9.0374134339102152	13.8569309599999944	F	F	F
1.3240724812970850	10.5436490062285841	12.5708101129999950	F	F	F
2.1038678492616638	10.5599920817428909	15.8638448872235198	T	T	T
3.2895529627197373	9.0863821983933377	15.8983928144118227	T	T	T
3.4613702730006852	10.5489144187452641	19.2245326665871161	T	T	T
3.4013549957314089	9.0389830135427314	17.8328272962433303	T	T	T
20.3035754017800372	9.0524572352212260	17.1737881273457198	T	T	T
4.7109793018690338	10.5403959877031355	15.8628821387454941	T	T	T
5.4736017942720192	10.5496435039310761	19.2687591010721491	T	T	T
0.1103452434537719	9.0525700286534292	19.0290960441964678	T	T	T
3.3796601406939342	9.0184127584140015	20.3341530202455090	T	T	T
1.2754336781327444	10.5560303558044417	19.2629605170775413	T	T	T
0.0000000000000014	13.5561201508653220	9.2861208469999976	F	F	F
0.0000000000000013	12.0498845785469495	7.9999999999999982	F	F	F
2.0578045142512522	13.5561201508653220	9.2861208469999976	F	F	F
3.3818769955483354	12.0498845785469495	9.2861208469999976	F	F	F
3.3818769955483354	13.5561201508653220	12.5708101129999950	F	F	F
3.3818769955483354	12.0498845785469495	11.2846892659999956	F	F	F
0.0000000000000014	12.0498845785469495	10.5722416939999970	F	F	F
4.7059494768454195	13.5561201508653220	9.2861208469999976	F	F	F
5.4396815097995868	13.5561201508653220	12.5708101129999950	F	F	F
0.0000000000000015	12.0498845785469495	12.5708101129999950	F	F	F
20.5011803087755169	13.5697203470390146	15.8031425244478445	T	T	T
0.0104583581408082	12.0610886164896165	14.6273039632873108	T	T	T
3.3818769955483354	12.0498845785469495	13.8569309599999944	F	F	F
1.3240724812970852	13.5561201508653220	12.5708101129999950	F	F	F
2.0625284395213614	13.5769531743071052	15.8485215337055276	T	T	T
3.4745669424956112	11.9608351804614106	15.8970590626915289	T	T	T
3.2634748556972673	13.5632095816869764	19.1736600447325038	T	T	T
3.3854302471114059	12.0610462889882086	17.8305198891516099	T	T	T
20.2943769385822570	12.0623865938309027	17.1736089503700242	T	T	T
4.7439786883598094	13.5482585177400363	15.8465791930986057	T	T	T
5.4954881995011151	13.5544948127602947	19.2634380933008167	T	T	T
-0.0366254660520790	12.0474161908973159	19.0288708883556730	T	T	T
3.3769652412287647	12.0729401104725262	20.3404115036838888	T	T	T
1.2804102307111724	13.5675298081344291	19.2494061890210837	T	T	T
6.7637539910966691	1.5062355723183694	9.2861208469999976	F	F	F
6.7637539910966691	0.0000000000000005	7.9999999999999982	F	F	F

8.8215585053479195	1.5062355723183694	9.2861208469999976	F	F	F
10.1456309866450027	0.0000000000000006	9.2861208469999976	F	F	F
10.1456309866450027	1.5062355723183696	12.5708101129999950	F	F	F
10.1456309866450027	0.0000000000000007	11.2846892659999956	F	F	F
6.7637539910966691	0.0000000000000007	10.5722416939999970	F	F	F
11.4697034679420877	1.5062355723183694	9.2861208469999976	F	F	F
12.2034355008962532	1.5062355723183696	12.5708101129999950	F	F	F
6.7637539910966691	0.0000000000000008	12.5708101129999950	F	F	F
6.6344135981482104	1.5103599971459218	15.8093465326340610	T	T	T
6.7647778258153153	-0.0020283807939723	14.6215792259148358	T	T	T
10.1456309866450027	0.0000000000000009	13.8569309599999944	F	F	F
8.0878264723937541	1.5062355723183696	12.5708101129999950	F	F	F
8.8045952336209794	1.4996765066289270	15.8464397650764734	T	T	T
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16.9093849777416700	3.0124711446367383	11.2846892659999956	F	F	F
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Oxide reference: TiO2(110)/fcc(111)_7x3sqrt3/Au E_tot= -3184.55683643 eV
 D3-zero damping= -49.0490118 eV, D3-BJ damping= -69.616517 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
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4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4
2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2
4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4
2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2
4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2
2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2
Selective dynamics
Cartesian
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  0.0000000000000008  0.0000000000000008 12.5708101129999967   F   F   F
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 13.5275079821933364 10.5436490062285841  9.2861208469999994   F   F   F
 13.5275079821933364  9.0374134339102152  8.0000000000000000   F   F   F
 15.5853124964445904 10.5436490062285841  9.2861208469999994   F   F   F
 16.9093849777416700  9.0374134339102152  9.2861208469999994   F   F   F
 16.9093849777416700 10.5436490062285841 12.5708101129999967   F   F   F
 16.9093849777416700  9.0374134339102152 11.2846892659999973   F   F   F
 13.5275079821933364  9.0374134339102152 10.5722416939999988   F   F   F
 18.2334574590387568 10.5436490062285841  9.2861208469999994   F   F   F
 18.9671894919929187 10.5436490062285841 12.5708101129999967   F   F   F
 13.5275079821933364  9.0374134339102152 12.5708101129999967   F   F   F
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 13.5086869083863554  9.0362233992148244 14.6051464010149452   T   T   T
 16.9093849777416700  9.0374134339102152 13.8569309599999961   F   F   F
 14.8515804634904178 10.5436490062285841 12.5708101129999967   F   F   F
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 13.5187077760591396  9.0325592350427630 18.9769778882385722   T   T   T
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 14.7791095918514888 10.5364502899509134 19.2772867510925501   T   T   T
 13.5275079821933364 13.5561201508653220  9.2861208469999994   F   F   F
 13.5275079821933364 12.0498845785469495  8.0000000000000000   F   F   F
 15.5853124964445904 13.5561201508653220  9.2861208469999994   F   F   F
 16.9093849777416700 12.0498845785469495  9.2861208469999994   F   F   F
 16.9093849777416700 13.5561201508653220 12.5708101129999967   F   F   F
 16.9093849777416700 12.0498845785469495 11.2846892659999973   F   F   F
 13.5275079821933364 12.0498845785469495 10.5722416939999988   F   F   F
 18.2334574590387568 13.5561201508653220  9.2861208469999994   F   F   F
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 13.5275079821933364 12.0498845785469495 12.5708101129999967   F   F   F
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 16.8865423247441555 12.0308646659864831 17.8443194076545026   T   T   T
 13.4949635863367021 12.0370259886136388 17.1372038739859605   T   T   T
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 13.4237531228495826 12.0446249929992906 18.9802508750672310   T   T   T
 16.8972852384053027 12.0518209592840826 20.3808746148885511   T   T   T
 14.7799424887619715 13.5577091622234818 19.2800538666160044   T   T   T

Metal reference: TiO2(110)/fcc(111)_7x3sqrt3/Au E_tot= -434.55123672 eV
 D3-zero damping= -54.3754143 eV, D3-BJ damping= -55.7450288 eV
Au
 1.0000000000000000
    20.2912619732900055    0.0000000000000012    0.0000000000000000
     0.0000000000000009   15.0623557231836873    0.0000000000000000
     0.0000000000000000    0.0000000000000000   35.3289349005892035
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 126
Cartesian
 19.2925227276590334  0.5632093338250228 22.3627116186775687
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 19.2938101855013429  3.9088998522174667 24.7772652430648925
 19.2963696952114034  2.2327543217937742 27.1985576522070183
 17.8446573547900122  3.0753719265262882 22.3550584452629799
 17.8469671889936770  4.7436069863562471 27.1993938676390137
 16.3960037309101452  0.5641199184811725 22.3656851093824578
 14.9475412386174984  1.3930065593549781 24.7816549371380610
 16.3976108282336952  3.9055100171661761 24.7799943710733857
 16.3979678784214364  2.2281916592398758 27.1974990363534950
 14.9464958923848830  3.0737420386304741 22.3592207000045420
 14.9482883394358268  4.7374089232202188 27.1981740834660144
 13.4952531910264426  0.5605363251627944 22.3694743867815369
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 13.4978707927146147  3.9038459196395263 24.7805398002092687
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 10.5966990734536015  0.5622610579934705 22.3691074670639338
  9.1489179006877563  1.3999913296780930 24.7851127255930095
 10.5993707848033161  3.9074553268435293 24.7838883148349645
 10.6006273936966178  2.2291974040622948 27.2013958102614239
  9.1500179499613150  3.0751378561331295 22.3593138362081412
  9.1489479887332319  4.7417343199732764 27.2017529720167417
  7.6998379227817084  0.5643277198272506 22.3660137352733521
  6.2490458770709481  1.4022924138347519 24.7792193404075221
  7.7011904634882598  3.9094178587536930 24.7783683386600693
  7.6996987494774691  2.2317613095064770 27.2005592147462032
  6.2507326294148529  3.0741176745603553 22.3545587414132960
  6.2514313031237041  4.7473668042030317 27.1936139799172949
  4.8012921349231030  0.5634057659911776 22.3599446924202354
  3.3512529243461540  1.4006106595751038 24.7765702155742922
  4.8031315054969630  3.9126288180329207 24.7727372226130313
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  3.3518976695934457  4.7465287571517374 27.1898586596701577
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  0.4534824381719715  1.4016247430816577 24.7775198568336421
  1.9006177344904662  3.9117504006160768 24.7712633487598346
  1.9025831697857705  2.2363638837081958 27.1931180498128349
  0.4512964051235951  3.0746211327806434 22.3524584421434369
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 19.2919494897251056  5.5841978897788662 22.3593670302170970
 17.8449940962811766  6.4205168622418958 24.7846717958890252
 19.2942862751472219  8.9337807808814080 24.7970717410527826
 19.2955887203058261  7.2535195084718884 27.2030056808797340
 17.8431672516378512  8.0958773594246978 22.3769034646718552
 17.8470446694643030  9.7605837382681244 27.2213101722127249
 16.3927549148544465  5.5848854412656888 22.3659979009449401
 14.9459569466912985  6.4183803199820364 24.7936908140944645
 16.3965909250625188  8.9317787675507709 24.8036357926827868
 16.3973028744752618  7.2496183863868007 27.2118046778688658
 14.9453612462678098  8.0955667568867433 22.3844163634477837
 14.9476645270190023  9.7597217182658582 27.2299553628121593
 13.4957504480563717  5.5846669297098250 22.3722617414949987
 12.0487810022952591  6.4195217849571247 24.7973499506986172
 13.4968835863794414  8.9315804151660476 24.8090944679794276
 13.4971662482206298  7.2500545166180999 27.2198639210656168
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 10.5994261477221485  5.5838106450680316 22.3702993420250671
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10.5962902460240969	8.9313361058769019	24.8050914789540364
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9.1482954806070040	8.0945000259844679	22.3783843240348084
9.1482696565767707	9.7616913788485711	27.2241362586527913
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7.6998627271671607	8.9342656760493266	24.8000244696023060
7.7010590555071881	7.2533903382932188	27.2041751254702540
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6.2501433376755235	9.7659734027215030	27.2197455818385592
4.8001555616454983	5.5849706273897768	22.3565122031806922
3.3521459812788232	6.4225465864468410	24.7799380371032676
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4.8024579819459507	7.2567636254939893	27.2040882929474641
3.3506399897435601	8.0945917160590515	22.3688253310657146
3.3538622589646523	9.7689257335017619	27.2117095365250030
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1.9019171381884803	8.9329490560770886	24.7914553107682814
1.9032052961269299	7.2574205022963447	27.2033169885836621
0.4498457567162698	8.0959799217639539	22.3713112287716420
0.4550103059094607	9.7658223630961540	27.2158986295675085
19.2921076522685802	10.6063880896181004	22.3819227394890703
17.8452966166738420	11.4429211022607547	24.8026894070520392
19.2975017939066227	13.9552513311235753	24.7900492057142223
19.2958685675004880	12.2749965266851468	27.2172234694637503
17.8431771515635447	13.1150635234288337	22.3777356925312318
17.8484414061178782	14.7824676333454406	27.2043640648061142
16.3929310557079937	10.6055879510205209	22.3877957542601997
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16.3963247762217925	13.9509077138343454	24.7955081123638443
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12.0463424263168886	11.4421199758227843	24.8126818941839105
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10.5977601561353616	13.9510792352969393	24.8007052721803873
10.5976887156735522	12.2721835181868570	27.2284323309942238
9.1478457459533153	13.1148696018601090	22.3806560645710881
9.1499481221330576	14.7845137834500573	27.2105017063768528
7.6999484252065233	10.6061455367480431	22.3848594641891765
6.2508987250516821	11.4443531691638967	24.8013034189038848
7.6994347511526122	13.9559335697645839	24.7928965374425871
7.7007226092448642	12.2750161503163540	27.2188726911871939
6.2486355559188294	13.1162886480120076	22.3770001181460465
6.2544461073259470	14.7873651285462859	27.2082231739587677
4.8003375374588417	10.6057995735636865	22.3828645692219261
3.3521489161012106	11.4439746216692537	24.8015254199628430
4.8016815878125492	13.9539195803970451	24.7933123049196773
4.8031607202496867	12.2791606094933439	27.2199298372919571
3.3498973589465804	13.1180827065499628	22.3774270526598293
3.3548683474779857	14.7908693791547385	27.2064758506032547
1.9016249989749856	10.6059695454794909	22.3812041913219808
0.4524373666624009	11.4440154047738414	24.7990939720474941
1.9023327570695501	13.9529181221806127	24.7950797043288631
1.9025911687892734	12.2790103971786007	27.2188921500487311

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  0.4518358581693770 13.1152509117242992 22.3761918473581254
  0.4517187655290834 14.7876483209665039 27.2089593094654880

Interface: TiO2(110)/fcc(111)_7x3sqrt3/Ag E_tot= -3564.15252219 eV
 D3-zero damping= -111.124575564 eV, D3-BJ damping= -136.881171745 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ag
 1.0000000000000000
    20.1636893636500041    0.0000000000000012    0.0000000000000000
     0.0000000000000009   14.9676576196619866    0.0000000000000000
     0.0000000000000000    0.0000000000000000   35.0809798297342041
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4
2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2
4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4
2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2
4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2
2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2 126
Selective dynamics
Cartesian
  0.0000000000000007  1.4967657619661994  9.2861208469999976   F   F   F
  0.0000000000000005  0.0000000000000005  7.9999999999999982   F   F   F
  2.0448669506656265  1.4967657619661994  9.2861208469999976   F   F   F
  3.3606148939416678  0.0000000000000006  9.2861208469999976   F   F   F
  3.3606148939416678  1.4967657619661996 12.5708101129999950   F   F   F
  3.3606148939416678  0.0000000000000007 11.2846892659999956   F   F   F
  0.0000000000000007  0.0000000000000007 10.5722416939999970   F   F   F
  4.6763628372177104  1.4967657619661994  9.2861208469999976   F   F   F
  5.4054818446072943  1.4967657619661996 12.5708101129999950   F   F   F
  0.0000000000000008  0.0000000000000008 12.5708101129999950   F   F   F
 20.0060443942694128  1.4947982526784662 15.8108283869760680   T   T   T
 -0.0053311745302938 -0.0026049536271131 14.6206986553749960   T   T   T
  3.3606148939416678  0.0000000000000009 13.8569309599999944   F   F   F
  1.3157479432760424  1.4967657619661996 12.5708101129999950   F   F   F
  2.0431208110754895  1.4862913780686202 15.8643616012942115   T   T   T
  3.3447518170317823  0.0075543806671073 15.8800298693236766   T   T   T
  3.4042468918054558  1.5051448982927043 19.1621461260919688   T   T   T
  3.3543418913098604 -0.0190106509568429 17.8454068279802804   T   T   T
 20.1639535134301582 -0.0004381877662370 17.1883723982934740   T   T   T
  4.6798159006618230  1.4877027791437019 15.8671443865834902   T   T   T
  5.4351617254102962  1.4967904459517656 19.2794378066500194   T   T   T
  0.0291171902427111  0.0054636907549394 19.0379683039207031   T   T   T
  3.3520287170740919  0.0271708163416473 20.3975501807880839   T   T   T
  1.2693584091611698  1.5003339335525696 19.2801354829545204   T   T   T
  0.0000000000000009  4.4902972858985972  9.2861208469999976   F   F   F
  0.0000000000000007  2.9935315239323979  7.9999999999999982   F   F   F
  2.0448669506656270  4.4902972858985972  9.2861208469999976   F   F   F
  3.3606148939416678  2.9935315239323979  9.2861208469999976   F   F   F
  3.3606148939416678  4.4902972858985972 12.5708101129999950   F   F   F
  3.3606148939416678  2.9935315239323983 11.2846892659999956   F   F   F
  0.0000000000000008  2.9935315239323979 10.5722416939999970   F   F   F
  4.6763628372177104  4.4902972858985972  9.2861208469999976   F   F   F
  5.4054818446072943  4.4902972858985972 12.5708101129999950   F   F   F
  0.0000000000000010  2.9935315239323983 12.5708101129999950   F   F   F
 19.9938233319720737  4.4931748502923989 15.8140570761807577   T   T   T
 -0.0162672992754098  2.9939329850146428 14.6230944957351916   T   T   T
  3.3606148939416678  2.9935315239323983 13.8569309599999944   F   F   F
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1.3157479432760426	4.4902972858985972	12.5708101129999950	F	F	F
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3.2009948521428457	2.9952434751191683	15.8628095188926981	T	T	T
3.4057438654210648	4.4840794503549564	19.1612113258166694	T	T	T
3.3576879338987937	2.9939264356649096	17.8247898788422532	T	T	T
20.1388584628840093	2.9930286918026319	17.1828811687451690	T	T	T
4.6783716297311200	4.4987503285367865	15.8664525160837275	T	T	T
5.4362735032493230	4.4902657034386673	19.2838448049467210	T	T	T
0.0050320406827278	2.9922026393078989	19.0302850168265714	T	T	T
3.3521292133270992	2.9939917185398675	20.3336800064198542	T	T	T
1.2681758085615491	4.4857828368869450	19.2838448760644958	T	T	T
0.0000000000000010	7.4838288098309951	9.2861208469999976	F	F	F
0.0000000000000009	5.9870630478647957	7.9999999999999982	F	F	F
2.0448669506656270	7.4838288098309951	9.2861208469999976	F	F	F
3.3606148939416682	5.9870630478647957	9.2861208469999976	F	F	F
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18.8479414203739637	7.4838288098309960	12.5708101129999950	F	F	F
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13.5235588993224987	7.4847684762947040	15.8019305725157011	T	T	T
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Oxide reference: TiO2(110)/fcc(111)_7x3sqrt3/Ag E_tot= -3187.95833681 eV
 D3-zero damping= -49.5211792 eV, D3-BJ damping= -70.4370148 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
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Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
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1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
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4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2
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Selective dynamics
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Metal reference: TiO2(110)/fcc(111)_7x3sqrt3/Ag E_tot= -354.00548931 eV
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  6.2157802499517798 14.6853887456114656 27.0243868735715260
  4.7758234115057983 10.5407928924202796 22.2759652375651882
  3.3337341768876421 11.3658212342751632 24.6509788128063434
  4.7747669354910744 13.8611842086076145 24.6505761407733637
  4.7751507610543857 12.1925164713292027 27.0248402328410293
  3.3339184591417315 13.0354190110729533 22.2760574624035748
  3.3342376570740631 14.6858172731326899 27.0300318887807158
  1.8923928195785449 10.5404167267173179 22.2765553038122199
  0.4516320517842007 11.3674118994986841 24.6494483964921862
  1.8930969633443890 13.8606494568606049 24.6516194241379303
  1.8931600529609567 12.1922857545911132 27.0246494320364121
  0.4537701408688778 13.0357916284985951 22.2724886369662904
  0.4540770898178584 14.6865242806669034 27.0269193576995477

Interface: TiO2(110)/fcc(111)_7x3sqrt3/Pt E_tot= -3988.05221507 eV
 D3-zero damping= -135.966898574 eV, D3-BJ damping= -157.752527988 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Pt
 1.0000000000000000
    19.3931735579400026    0.0000000000000012    0.0000000000000000
     0.0000000000000009   14.3956979667228762    0.0000000000000000
     0.0000000000000000    0.0000000000000000   35.3385814848379951
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4
2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2
4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4
2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2
4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2
2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2 126
Selective dynamics
Cartesian
  0.0000000000000006  1.4395697966722885  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  7.9999999999999991   F   F   F
  1.9667263744225560  1.4395697966722885  9.2861208469999994   F   F   F
  3.2321955929900006  0.0000000000000006  9.2861208469999994   F   F   F
  3.2321955929900006  1.4395697966722887 12.5708101129999967   F   F   F
  3.2321955929900006  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416939999988   F   F   F
  4.4976648115574465  1.4395697966722885  9.2861208469999994   F   F   F
  5.1989219674125566  1.4395697966722887 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 19.3971595033226656  1.5078046706270694 15.9303257536989538   T   T   T
  0.0052926473678653  0.0013757884986801 14.6011060733942433   T   T   T
  3.2321955929900006  0.0000000000000008 13.8569309599999961   F   F   F
  1.2654692185674457  1.4395697966722887 12.5708101129999967   F   F   F
  1.9617274335172858  1.4325654258780913 15.8773874718462480   T   T   T
  3.2342905612323469 -0.0002024854172726 15.9012318114407076   T   T   T
```

3.2436278577522026	1.4583219762300754	19.1760743005216341	T	T	T
3.2256210173876552	-0.0119500138633537	17.8893374379774421	T	T	T
19.3955536187140325	-0.0078529577778901	17.2257875675763046	T	T	T
4.5127178680429596	1.4279126116345091	15.8763753485091303	T	T	T
5.2228545200713699	1.4562065860742708	19.3148568985936322	T	T	T
-0.0121970412813017	0.0542699851544498	19.0677320501032561	T	T	T
3.3141300590752905	0.0976147581387191	20.5568207641281973	T	T	T
1.2681354976628370	1.4467295391610593	19.3667709014533287	T	T	T
0.0000000000000008	4.3187093900168643	9.2861208469999994	F	F	F
0.0000000000000007	2.8791395933445760	7.9999999999999991	F	F	F
1.9667263744225563	4.3187093900168643	9.2861208469999994	F	F	F
3.2321955929900006	2.8791395933445760	9.2861208469999994	F	F	F
3.2321955929900006	4.3187093900168643	12.5708101129999967	F	F	F
3.2321955929900006	2.8791395933445765	11.2846892659999973	F	F	F
0.0000000000000008	2.8791395933445760	10.5722416939999988	F	F	F
4.4976648115574465	4.3187093900168643	9.2861208469999994	F	F	F
5.1989219674125566	4.3187093900168643	12.5708101129999967	F	F	F
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19.3967812320486104	4.2568292358954851	15.9305721480722386	T	T	T
0.0048313563215518	2.8817181070944988	14.5976037677441184	T	T	T
3.2321955929900006	2.8791395933445765	13.8569309599999961	F	F	F
1.2654692185674459	4.3187093900168643	12.5708101129999967	F	F	F
1.9616199336156304	4.3316707459549324	15.8731240831867026	T	T	T
3.2409474968995151	2.8836402415307250	15.8763362821443543	T	T	T
3.2447480241455047	4.3289439925677389	19.1634979061467732	T	T	T
3.2430364336011595	2.8823136953728978	17.8418712520591960	T	T	T
19.4039640414519212	2.8830131060902113	17.1900361584708321	T	T	T
4.5128228321408521	4.3371308701209230	15.8771699090433778	T	T	T
5.2284336082674230	4.3067365907993942	19.2899420723711330	T	T	T
0.0700223481187779	2.8902934493573613	19.8773713455339731	T	T	T
3.2356978696724124	2.8970361647682572	20.4374519772318166	T	T	T
1.2720422776300233	4.3351713505778182	19.3786429658582762	T	T	T
0.0000000000000010	7.1978489833614399	9.2861208469999994	F	F	F
0.0000000000000008	5.7582791866891521	7.9999999999999991	F	F	F
1.9667263744225565	7.1978489833614399	9.2861208469999994	F	F	F
3.2321955929900010	5.7582791866891521	9.2861208469999994	F	F	F
3.2321955929900010	7.1978489833614399	12.5708101129999967	F	F	F
3.2321955929900010	5.7582791866891521	11.2846892659999973	F	F	F
0.0000000000000010	5.7582791866891521	10.5722416939999988	F	F	F
4.4976648115574465	7.1978489833614399	9.2861208469999994	F	F	F
5.1989219674125566	7.1978489833614399	12.5708101129999967	F	F	F
0.0000000000000011	5.7582791866891521	12.5708101129999967	F	F	F
19.3978150235318125	7.1748140281516699	15.7986134896690125	T	T	T
0.0045733795287098	5.7627438168247158	14.6006336964201715	T	T	T
3.2321955929900010	5.7582791866891521	13.8569309599999961	F	F	F
1.2654692185674461	7.1978489833614399	12.5708101129999967	F	F	F
1.9545431235265924	7.2192551757090513	15.8993064767342176	T	T	T
3.2332990189554436	5.7678650955995430	15.8907263525792910	T	T	T
3.2465374969303618	7.1753476716363647	19.2913951476461101	T	T	T
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-0.0097358657949234	5.7221784279189682	19.0658391740985493	T	T	T
3.3753874084012025	5.6838826965378848	20.5173763747512865	T	T	T
1.2613606188436968	7.1679158085039862	19.4159161324075988	T	T	T
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0.0000000000000010	8.6374187800337285	7.9999999999999991	F	F	F
1.9667263744225567	10.0769885767060163	9.2861208469999994	F	F	F
3.2321955929900010	8.6374187800337285	9.2861208469999994	F	F	F
3.2321955929900010	10.0769885767060163	12.5708101129999967	F	F	F
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4.4976648115574474	10.0769885767060163	9.2861208469999994	F	F	F
5.1989219674125575	10.0769885767060163	12.5708101129999967	F	F	F
0.0000000000000013	8.6374187800337285	12.5708101129999967	F	F	F
19.3929880820450400	10.0807254603763425	15.9039355327191743	T	T	T
0.0029676102431351	8.6625022566658938	14.6233071206901268	T	T	T
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1.2654692185674461	10.0769885767060163	12.5708101129999967	F	F	F
1.9571340700444302	10.0830025378090475	15.9264626787668337	T	T	T
3.2389720536205493	8.6458125157591752	16.0141645601020208	T	T	T
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3.2457379992236834	8.6666970931678886	17.9639716281745301	T	T	T
19.4176376926169851	8.6373967162163048	17.2718129520935690	T	T	T
4.5188136366988143	10.0823930149928849	15.9147152386388981	T	T	T
5.2300454525485973	10.0844383388767493	19.4615913170212984	T	T	T
0.0175950042746965	8.6256438616826561	19.1279928389309042	T	T	T
3.2368367553374493	8.5739279512113615	20.5824127942880679	T	T	T
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4.4976648115574474	12.9561281700505919	9.2861208469999994	F	F	F
5.1989219674125575	12.9561281700505919	12.5708101129999967	F	F	F
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19.3977464546205738	12.9860226817126918	15.8001265413802319	T	T	T
0.0039077452908083	11.4991842707230525	14.6236682230874813	T	T	T
3.2321955929900015	11.5165583733783023	13.8569309599999961	F	F	F
1.2654692185674463	12.9561281700505919	12.5708101129999967	F	F	F
1.9551641517226699	12.9451831606647936	15.9059629126656255	T	T	T
3.2408144425191550	11.5175570188735854	16.0089042455331665	T	T	T
3.2438367309828902	12.9937992952691452	19.2975294869562468	T	T	T
3.2461659888571663	11.5118521622240149	17.9686753801029049	T	T	T
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5.2318761437141239	12.9914387015331396	19.3927095177664555	T	T	T
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9.6965867789700013	0.0000000000000006	9.2861208469999994	F	F	F
9.6965867789700013	1.4395697966722887	12.5708101129999967	F	F	F
9.6965867789700013	0.0000000000000007	11.2846892659999973	F	F	F
6.4643911859800012	0.0000000000000006	10.5722416939999988	F	F	F
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6.4643911859800012	0.0000000000000007	12.5708101129999967	F	F	F
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9.6930168851079781	-0.0019870999890811	15.9048471171901209	T	T	T
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10.9707802405840944	1.4362079350278629	15.8719420872397929	T	T	T
11.6914326537123880	1.4657523795410239	19.3803066841944975	T	T	T
6.4936089755076933	0.0513634085081416	19.0609752703092106	T	T	T

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8.4311175604025568	4.3187093900168643	9.2861208469999994	F	F	F
9.6965867789700013	2.8791395933445760	9.2861208469999994	F	F	F
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6.4643911859800012	2.8791395933445760	10.5722416939999988	F	F	F
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9.6965867789700013	5.7582791866891521	9.2861208469999994	F	F	F
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9.6965867789700013	5.7582791866891521	13.8569309599999961	F	F	F
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9.6813109006531608	5.7669521007484335	17.8907549852785870	T	T	T
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8.4311175604025586	10.0769885767060163	9.2861208469999994	F	F	F
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10.9620559975374459	10.0769885767060163	9.2861208469999994	F	F	F
11.6633131533925578	10.0769885767060163	12.5708101129999967	F	F	F
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Oxide reference: TiO2(110)/fcc(111)_7x3sqrt3/Pt E_tot= -3186.10757485 eV
 D3-zero damping= -52.543609 eV, D3-BJ damping= -75.5587516 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
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2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2
4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4
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4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2
2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2
Selective dynamics
Cartesian
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  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
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  3.2321955929900006  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416939999988   F   F   F
  4.4976648115574465  1.4395697966722885  9.2861208469999994   F   F   F
  5.1989219674125566  1.4395697966722887 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 19.3943452485792704  1.4427242879530195 15.8352270793156737   T   T   T
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Metal reference: TiO2(110)/fcc(111)_7x3sqrt3/Pt E_tot= -777.7997133 eV
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Interface: TiO2(110)/fcc(111)_7x3sqrt3/Pd E_tot= -3863.21525995 eV
 D3-zero damping= -122.728103637 eV, D3-BJ damping= -150.16671421 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Pd
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    19.2358686233000036    0.0000000000000012    0.0000000000000000
     0.0000000000000009   14.2789293356895417    0.0000000000000000
     0.0000000000000000    0.0000000000000000   35.0369793684969153
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1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4
2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2
4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4
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2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2 126
Selective dynamics
Cartesian
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  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
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  3.2059781038833344  1.4278929335689550 12.5708101129999967   F   F   F
  3.2059781038833344  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416939999988   F   F   F
  4.4611826511157373  1.4278929335689547  9.2861208469999994   F   F   F
  5.1567516605342654  1.4278929335689550 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 19.2344548987640671  1.4973122419870553 15.9394523523694058   T   T   T
  0.0022212372026558  0.0055221534372108 14.5981441413843562   T   T   T
  3.2059781038833344  0.0000000000000008 13.8569309599999961   F   F   F
  1.2552045472324036  1.4278929335689550 12.5708101129999967   F   F   F
  1.9382104944132130  1.4164376930846234 15.8863683857933538   T   T   T
  3.2062161926293147 -0.0035357037545893 15.9482550979865838   T   T   T
  3.2053055478876704  1.4493480557047544 19.2120934826391689   T   T   T
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  4.4740988547546712  1.4166273416384347 15.8869296142774932   T   T   T
  5.1725365700350414  1.4471435776972861 19.4120838267489013   T   T   T
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  0.0057048072179174  2.8581824756475451 14.5986289659912263   T   T   T
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  3.2047084941694939  2.8548662157937605 17.8550610123618121   T   T   T
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6.4335331721746991	0.0637556293773082	19.0835801551395150	T	T	T
9.6251073693342040	0.0274612296441790	20.5298494820424260	T	T	T
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9.6179343116500018	2.8557858671379086	9.2861208469999994	F	F	F
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9.6179343116500018	2.8557858671379091	11.2846892659999973	F	F	F
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16.0298905194166679	2.8557858671379091	11.2846892659999973	F	F	F
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Oxide reference: TiO2(110)/fcc(111)_7x3sqrt3/Pd E_tot= -3179.69099386 eV
 D3-zero damping= -53.1806391 eV, D3-BJ damping= -76.6224942 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
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     0.0000000000000009   14.2789293356895417    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6667175344326068
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4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4
2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2
4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4
2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2
4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2
2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2
Selective dynamics
Cartesian
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  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
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  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
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  1.2552045472324036  1.4278929335689550 12.5708101129999967   F   F   F
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 16.0291667318946054  5.7118436706581095 17.9899674398214628   T   T   T
 12.8252737637354670  5.7126127916547143 17.2542439144479047   T   T   T
 17.3111102624165660  7.1395083859350343 15.9368733478362845   T   T   T
 18.0209602665811808  7.1398057958014025 19.4806441563075232   T   T   T
 12.8246568707201209  5.7116812587496613 19.0854825132092323   T   T   T
 16.0321332499914035  5.7131603146179808 20.6636254880078454   T   T   T
 14.0403580383245412  7.1396380031932347 19.4811782564965164   T   T   T
 12.8239124155333357  9.9952505349826826  9.2861208469999994   F   F   F
 12.8239124155333357  8.5673576014137272  8.0000000000000000   F   F   F
 14.7746859721842689  9.9952505349826826  9.2861208469999994   F   F   F
 16.0298905194166679  8.5673576014137272  9.2861208469999994   F   F   F
 16.0298905194166679  9.9952505349826826 12.5708101129999967   F   F   F
 16.0298905194166679  8.5673576014137272 11.2846892659999973   F   F   F
 12.8239124155333357  8.5673576014137272 10.5722416939999988   F   F   F
 17.2850950666490739  9.9952505349826826  9.2861208469999994   F   F   F
 17.9806640760675975  9.9952505349826826 12.5708101129999967   F   F   F
 12.8239124155333357  8.5673576014137272 12.5708101129999967   F   F   F
 12.8248565763296476  9.9958262163797205 15.8436297605183789   T   T   T
 12.8249751230753457  8.5684197914064697 14.6194692570633862   T   T   T
 16.0298905194166679  8.5673576014137272 13.8569309599999961   F   F   F
 14.0791169627657347  9.9952505349826826 12.5708101129999967   F   F   F
 14.7502716911746159  9.9959509063979759 15.9377243179026404   T   T   T
 16.0311215222231631  8.5677746457829489 16.1030596187510220   T   T   T
 16.0312997957354284  9.9955760658423607 19.5090473511240923   T   T   T
 16.0321453647049097  8.5678423587141648 17.9882735014676634   T   T   T
 12.8244184826676939  8.5673203276449836 17.2546959304991603   T   T   T
 17.3111584789701887  9.9958606676238109 15.9344248730375266   T   T   T
 18.0213592409063565  9.9956771375327467 19.4829817338405213   T   T   T
 12.8244707501304518  8.5674667894466765 19.0859655305833620   T   T   T
 16.0294807065413423  8.5681406192574450 20.6615399841914531   T   T   T
 14.0409003691592176  9.9956637421829697 19.4785709351437895   T   T   T
 12.8239124155333357 12.8510364021205898  9.2861208469999994   F   F   F
 12.8239124155333357 11.4231434685516327  8.0000000000000000   F   F   F
 14.7746859721842689 12.8510364021205898  9.2861208469999994   F   F   F
 16.0298905194166679 11.4231434685516327  9.2861208469999994   F   F   F
 16.0298905194166679 12.8510364021205898 12.5708101129999967   F   F   F
 16.0298905194166679 11.4231434685516327 11.2846892659999973   F   F   F
 12.8239124155333357 11.4231434685516327 10.5722416939999988   F   F   F
 17.2850950666490739 12.8510364021205898  9.2861208469999994   F   F   F
 17.9806640760675975 12.8510364021205898 12.5708101129999967   F   F   F
 12.8239124155333357 11.4231434685516327 12.5708101129999967   F   F   F
 12.8248560598671606 12.8515731672345321 15.8425327928100046   T   T   T
 12.8251859696842256 11.4233779531679058 14.6194231292342884   T   T   T
 16.0298905194166679 11.4231434685516327 13.8569309599999961   F   F   F
 14.0791169627657347 12.8510364021205898 12.5708101129999967   F   F   F
 14.7503998031512609 12.8517910474794501 15.9366933095077972   T   T   T
 16.0310104330848837 11.4238193025221317 16.1037208225954629   T   T   T
 16.0310301301859965 12.8514348745560891 19.5108247160763035   T   T   T
 16.0327877697626313 11.4240332754724374 17.9885677923743792   T   T   T
 12.8240646119779047 11.4246346986712837 17.2546096594870804   T   T   T
 17.3110931916719544 12.8522822191592727 15.9366973005560961   T   T   T
 18.0214704870033948 12.8516146448121784 19.4819722737333798   T   T   T
 12.8248684062184655 11.4235282262227944 19.0859109275827592   T   T   T
 16.0293369295570649 11.4231489764516798 20.6618152958155044   T   T   T
 14.0408974558790405 12.8517313752323421 19.4798847033282350   T   T   T

Metal reference: TiO2(110)/fcc(111)_7x3sqrt3/Pd E_tot= -656.32945025 eV
 D3-zero damping= -45.6811505 eV, D3-BJ damping= -56.1675948 eV
Pd
 1.0000000000000000
    19.2358686233000036    0.0000000000000012    0.0000000000000000
     0.0000000000000009   14.2789293356895417    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.5857170335691144
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 126
Cartesian
 18.2946966984142030  0.5236643335819772  8.0106212274683752
 16.9238811688571928  1.3224528672654192 10.2942376587730724
 18.2984050702378767  3.7034206549275051 10.2875566864081627
 18.2986808863192181  2.1233722301490583 12.5662619704055789
 16.9211265063880276  2.9021487409664184  8.0156218661635474
 16.9253093722390595  4.5042834491380397 12.5724870484349811
 15.5470398076705063  0.5203602685432694  8.0226870388530465
 14.1753429031991534  1.3189636796623398 10.3049885319599692
 15.5502733392249333  3.7006403845244167 10.2996988647856700
 15.5500637076520878  2.1208044550302874 12.5791345538954857
 14.1734318313335148  2.9017108310717137  8.0264701124587656
 14.1771806635718995  4.5006770400430449 12.5828489824382377
 12.8010563214869464  0.5198936160178921  8.0264667924294102
 11.4279274776330926  1.3196083041699302 10.3040916544567160
 12.8013187861125992  3.6995041493277445 10.3068528747243349
 12.8013081444937100  2.1199742128049963 12.5857027792667910
 11.4277614981408444  2.9008563375900165  8.0260608100394943
 11.4279994112060077  4.5008578375325223 12.5842695314767781
 10.0543510927574342  0.5206616715344714  8.0219913281301043
  8.6791299084306299  1.3221103625803441 10.2935786311893462
 10.0528489510389605  3.7017917614183786 10.2998984128539597
 10.0536980895886323  2.1213432135044226 12.5775104134295006
  8.6813066678680908  2.9036949243698285  8.0145193480130139
  8.6782756084876134  4.5034410130349309 12.5734318265333727
  7.3065384958655839  0.5228039928950311  8.0109888385455879
  5.9300862115286046  1.3254879478174162 10.2833926834752454
  7.3042017804837416  3.7048045673227619 10.2867862370443408
  7.3049578489196838  2.1246765396741090 12.5645991905028289
  5.9326206942748705  2.9051011875163555  8.0029285096716549
  5.9302609539441296  4.5067311427571521 12.5624669345850091
  4.5570387708928486  0.5258274714109435  8.0036446886758181
  3.1826560855130741  1.3269200010834492 10.2811978181603152
  4.5567279911284606  3.7072479738687543 10.2797566439079748
  4.5571560990712818  2.1268657737034791 12.5587280778634938
  3.1825664350633498  2.9052731283919471  8.0000715895685328
  3.1828650549504784  4.5056906643489878 12.5567859066858247
  1.8083051939371526  0.5260957456884564  8.0023804037295037
  0.4357343849332612  1.3256329193091578 10.2835212719011722
  1.8099802468992172  3.7064216351593982 10.2781132028273614
  1.8098321295509927  2.1266283043181433 12.5595316445762162
  0.4339815957111842  2.9039458335757704  8.0031048137917153
  0.4362152102880537  4.5046140515347863 12.5617973575151378
 18.2973669655611353  5.2828748495923827  8.0093070910342714
 16.9256040452010446  6.0817739910940380 10.2941233762112176
 18.2982424209346419  8.4638691204957706 10.2931132295153684
 18.3003502611425013  6.8839741566431485 12.5703837795160762
 16.9235273153000918  7.6615741122113317  8.0175873541147311
 16.9255687004757220  9.2634895909077795 12.5762475911639928
 15.5491650328202908  5.2800335322065548  8.0195987787705310
 14.1772267485435126  6.0782340785463020 10.3012990198859260
 15.5501465132006373  8.4589856610030392 10.3000933975399498
 15.5523935859621805  6.8815253557336336 12.5779003709828636
 14.1758882353579470  7.6603799531758661  8.0223753511992442
 14.1763745819718157  9.2590208397205362 12.5808365848133885
 12.8007458965766734  5.2809790387437348  8.0265406284056837
 11.4282587826897917  6.0789474448749843 10.3028290546383090
 12.8022464760747674  8.4583505267509498 10.3015407729300570
 12.8029511752242229  6.8798975842821593 12.5806977890663525
 11.4272999445274426  7.6607037112829044  8.0222527436343078
 11.4281537171058059  9.2583921426753886 12.5807295165958681
 10.0534259505809800  5.2825434243072902  8.0215867482785299
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8.6783532688458944	6.0819786525717578	10.2951906430434654
10.0542193195959406	8.4600094681035660	10.3001766514733895
10.0537542755769191	6.8802622438392076	12.5779766855984203
8.6792715779033429	7.6635328941830094	8.0181028670347825
8.6794479382575371	9.2600812215081305	12.5779333111992511
7.3056366083914384	5.2827832643905142	8.0088462092393407
5.9305410112428065	6.0854267395893897	10.2848443824198323
7.3059849339124732	8.4641172594989680	10.2933981341504452
7.3039502567713885	6.8836477002356284	12.5690401883249070
5.9311505272202734	7.6658528733992588	8.0096654278057215
5.9311459820445496	9.2651487951800462	12.5691649408593467
4.5573241325176888	5.2850772803338320	8.0008652485628122
3.1828978291101353	6.0867644507839938	10.2802959745435221
4.5576005040702539	8.4672497987441950	10.2867586772905391
4.5561874462241505	6.8852026419162113	12.5624338681677887
3.1834008306698349	7.6657719875705999	8.0039538077451802
3.1839813970584627	9.2672975253752181	12.5648082771572369
1.8089357423816133	5.2856944613162220	8.0001147376532664
0.4369435492563661	6.0847110184744722	10.2858222177893666
1.8105441439743797	8.4675867449001441	10.2853555434325461
1.8108156629980516	6.8862213209208516	12.5622580621004865
0.4356175207791332	7.6644723789961482	8.0094267230775795
0.4373831783364222	9.2665978916344347	12.5680134397366565
18.2976288977930146	10.0438390580086008	8.0151795382393907
16.9235539446440555	10.8420977429147598	10.2988104250507497
18.2970500813595081	13.2235544493607531	10.2913548214578565
18.2991228743829026	11.6453695793127707	12.5734167761239579
16.9220532641538277	12.4203470113692998	8.0185707604443301
16.9234646883838806	14.0222118024324214	12.5739661739059461
15.5499066856735819	10.0399649152268005	8.0218892368842383
14.1755982038782662	10.8384293589509539	10.3024183347708256
15.5488982022993909	13.2188952817570051	10.3009850653506181
15.5503151445688346	11.6412932652620924	12.5807241240315886
14.1748091821697066	12.4193061893587462	8.0246018447324445
14.1739971001222891	14.0187295862328227	12.5834157131739008
12.8013643743872585	10.0390859998603279	8.0231575705217342
11.4283813052760461	10.8380659196527063	10.3032664293031608
12.8014898925369547	13.2172681042723834	10.3050733637338023
12.8014964004730345	11.6367297403956140	12.5838044631392361
11.4280696048193864	12.4196245807700638	8.0257234789437053
11.4266419368131640	14.0182827669235426	12.5822870297053786
10.0543134203356299	10.0413906031839009	8.0217271126268823
8.6804748720056200	10.8407079037828744	10.2990046804766013
10.0537152990565790	13.2185029589153036	10.3010104240416975
10.0540030819172923	11.6386558424218496	12.5806327156571509
8.6803861955163004	12.4209075708098204	8.0189155969747468
8.6802830915683540	14.0214080492620816	12.5753121799462324
7.3049257569600847	10.0432717833735818	8.0164799108629481
5.9312828481091318	10.8458527395369977	10.2904303331276505
7.3055732229941626	13.2225677550532144	10.2924261279783558
7.3054915113069274	11.6444297857400318	12.5732581304237865
5.9320293686986965	12.4237841956661494	8.0092618116780532
5.9323677048922594	14.0253147024737945	12.5657234158064828
4.5562616396265767	10.0465865986699079	8.0077052271749558
3.1831605481660583	10.8480287472378905	10.2852660145139119
4.5573190744136296	13.2259278212622569	10.2856712746820058
4.5583209087476311	11.6462248256587255	12.5665759255441500
3.1824557723292677	12.4265015153263469	8.0046072754157418
3.1844730349639145	14.0261235922313485	12.5620140981451804
1.8088020833478919	10.0464411384336856	8.0063539244187893
0.4357372752968211	10.8469668485680497	10.2890599922026169
1.8098244568029003	13.2265543871575755	10.2828549395085904
1.8111854381259154	11.6468408812314923	12.5629403097917347

```
  0.4342821226427445 12.4252589438556136  8.0076520048870901
  0.4372875565720823 14.0250285746585881 12.5650381585693900

Interface: TiO2(110)/fcc(111)_7x3sqrt3/Ir E_tot= -4285.47530313 eV
 D3-zero damping= -130.342294808 eV, D3-BJ damping= -155.90423788 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ir
 1.0000000000000000
    19.0054425018500055    0.0000000000000012    0.0000000000000000
     0.0000000000000009   14.1078823000856417    0.0000000000000000
     0.0000000000000000    0.0000000000000000   35.0918050195080582
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4
2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2
4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4
2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2
4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2
2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2 126
Selective dynamics
Cartesian
  0.0000000000000006  1.4107882300085650  9.2861208470000012   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000018   F   F   F
  1.9274052755876161  1.4107882300085650  9.2861208470000012   F   F   F
  3.1675737503083350  0.0000000000000005  9.2861208470000012   F   F   F
  3.1675737503083350  1.4107882300085652 12.5708101129999985   F   F   F
  3.1675737503083350  0.0000000000000007 11.2846892659999991   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.4077422250290548  1.4107882300085650  9.2861208470000012   F   F   F
  5.0949790258959506  1.4107882300085652 12.5708101129999985   F   F   F
  0.0000000000000007  0.0000000000000007 12.5708101129999985   F   F   F
 19.0053650365533287  1.4632319190184711 15.9943676866992401   T   T   T
 -0.0048940065104055 -0.0159982732225648 14.6179819338775445   T   T   T
  3.1675737503083350  0.0000000000000008 13.8569309599999979   F   F   F
  1.2401684747207198  1.4107882300085652 12.5708101129999985   F   F   F
  1.9199907841102508  1.3703304800293312 15.9543268328967258   T   T   T
  3.1672639308752495 -0.0402725588866167 15.7932415711934713   T   T   T
  3.1638526872629660  1.4336182013597349 19.2112295031208333   T   T   T
  3.1618903794912629 -0.0641037804296278 18.0836363659360941   T   T   T
 19.0052854368261315 -0.0259620590897838 17.3002749227927808   T   T   T
  4.4127633329762013  1.3711321574934967 15.9584246023028946   T   T   T
  5.1023093469474405  1.4326043546920202 19.5219166421988568   T   T   T
 -0.0199068796912421  0.0737651752682096 19.1322142178776637   T   T   T
  3.1729211593986242  0.1915599053913192 20.8161128577376182   T   T   T
  1.2256610304786024  1.4300006147883888 19.5293214662997379   T   T   T
  0.0000000000000008  4.2323646900256939  9.2861208470000012   F   F   F
  0.0000000000000006  2.8215764600171291  8.0000000000000018   F   F   F
  1.9274052755876163  4.2323646900256939  9.2861208470000012   F   F   F
  3.1675737503083350  2.8215764600171291  9.2861208470000012   F   F   F
  3.1675737503083350  4.2323646900256939 12.5708101129999985   F   F   F
  3.1675737503083350  2.8215764600171296 11.2846892659999991   F   F   F
  0.0000000000000008  2.8215764600171291 10.5722416940000006   F   F   F
  4.4077422250290548  4.2323646900256939  9.2861208470000012   F   F   F
  5.0949790258959506  4.2323646900256939 12.5708101129999985   F   F   F
  0.0000000000000009  2.8215764600171296 12.5708101129999985   F   F   F
 19.0026902317952207  4.1604609463065474 15.9324560674400573   T   T   T
  0.0041424019315739  2.7928051435054773 14.6108161821908986   T   T   T
  3.1675737503083350  2.8215764600171296 13.8569309599999979   F   F   F
```

1.2401684747207200	4.2323646900256939	12.5708101129999985	F	F	F
1.9158839708489410	4.2504597677241147	15.9081743936273430	T	T	T
3.1660584392917923	2.8192136012175437	15.8856145109957811	T	T	T
3.1635584109413375	4.1956160279534016	19.3730927166227325	T	T	T
3.1629004558160059	2.8465162509657196	17.9363338060551492	T	T	T
18.9966099686958820	2.8304470176055068	17.2292034328538364	T	T	T
4.4158798295195707	4.2505341751088093	15.9113958018899808	T	T	T
5.1030743518208750	4.1975164128208817	19.5092424039530705	T	T	T
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15.8378687515416718	2.8215764600171291	9.2861208470000012	F	F	F
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12.6702950012333382	2.8215764600171296	12.5708101129999985	F	F	F
12.6689384182931466	4.2609078979213866	15.8382280206271933	T	T	T
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13.9104634759540549	4.2323646900256939	12.5708101129999985	F	F	F
14.5932260441901764	4.2233584376178888	15.9038806570399434	T	T	T
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Oxide reference: TiO2(110)/fcc(111)_7x3sqrt3/Ir E_tot= -3165.96106486 eV
 D3-zero damping= -54.0961997 eV, D3-BJ damping= -78.1321807 eV
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Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
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Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
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Selective dynamics
Cartesian
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Metal reference: TiO2(110)/fcc(111)_7x3sqrt3/Ir E_tot= -1094.43475614 eV
 D3-zero damping= -55.8598877 eV, D3-BJ damping= -60.9253372 eV
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  9.9397103587145086 13.1006885727770115 24.9005775777084644
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  8.5837129671241978 12.3167314841198365 22.7249692865689248
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  7.2263854430631493  9.9658682106320420 22.7233009105313819
  5.8674241264549325 10.7498833912737801 24.8956133099511945
  7.2249557847624999 13.1011689218800136 24.8974741499486285
  7.2234289876059261 11.5337731155303160 27.0712429777306340
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  5.8664522366633953 13.8853996314340442 27.0701985453950194
  4.5106205421245109  9.9663936817196479 22.7208207267250479
  3.1522539466042105 10.7504469006750174 24.8940856728554394
  4.5100262797108606 13.1016352159009717 24.8947455023454758
  4.5091574627956410 11.5343933213965268 27.0687030728449045
  3.1522770432554585 12.3180774937150659 22.7209002095914840
  3.1525404734284344 13.8857608212706900 27.0689728870285649
  1.7943437885827882  9.9664488244992651 22.7210160345256895
  0.4371893550201597 10.7499309498125655 24.8962444871959114
  1.7946658318586219 13.1015376482528598 24.8955068995791713
  1.7954805699883813 11.5340804243842481 27.0691156768531904
  0.4361463525564979 12.3174664067459680 22.7228241924378729
  0.4381099885974365 13.8855346161638931 27.0709370979643360

Interface: TiO2(110)/fcc(111)_7x3sqrt3/Rh E_tot= -4071.308539 eV
 D3-zero damping= -120.61609248 eV, D3-BJ damping= -149.205624394 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Rh
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    18.7436388669600049    0.0000000000000011    0.0000000000000000
     0.0000000000000009   13.9135435012703432    0.0000000000000000
     0.0000000000000000    0.0000000000000000   35.0099083997701825
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4
2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2
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2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2
4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2
2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2 126
Selective dynamics
Cartesian
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  0.0000000000000005  0.0000000000000005  7.9999999999999991   F   F   F
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  3.1239398111600014  0.0000000000000005  9.2861208469999994   F   F   F
  3.1239398111600014  1.3913543501270353 12.5708101129999967   F   F   F
  3.1239398111600014  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416939999988   F   F   F
  4.3470247260253654  1.3913543501270351  9.2861208469999994   F   F   F
  5.0247947074546389  1.3913543501270353 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000007 12.5708101129999967   F   F   F
 18.7346362404352718  1.4544442739436529 16.0917348714998774   T   T   T
 -0.1005515543143838 -0.0081029436992801 14.6872570641599047   T   T   T
  3.1239398111600014  0.0000000000000008 13.8569309599999961   F   F   F
  1.2230849148653642  1.3913543501270353 12.5708101129999967   F   F   F
  1.9209787748189235  1.3452417021892060 15.9791405104031252   T   T   T
  3.1857361525814030 -0.0613793772419089 15.7542874106823874   T   T   T
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3.2033273049260154	1.4090917722974072	19.3427008256775430	T	T	T
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4.3361681999360275	1.4011555790994494	16.1645901240808954	T	T	T
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3.2966584513373993	0.2110124325748226	21.0189022152819334	T	T	T
1.2502997889418588	1.4558294370788307	19.8800085074103201	T	T	T
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1.9008548962946383	4.1740630503811040	9.2861208469999994	F	F	F
3.1239398111600014	2.7827087002540694	9.2861208469999994	F	F	F
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3.0222641732787547	2.8560633904787807	18.1787841367711174	T	T	T
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5.0801496236296382	4.2528016904430821	19.4729024312448189	T	T	T
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6.2478796223200037	8.3481261007622081	10.5722416939999988	F	F	F
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15.6196990558000053	8.3481261007622081	9.2861208469999994	F	F	F
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Oxide reference: TiO2(110)/fcc(111)_7x3sqrt3/Rh E_tot= -3144.77598412 eV
 D3-zero damping= -55.2120188 eV, D3-BJ damping= -79.9472006 eV
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O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
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O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
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4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4
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Cartesian
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9.3718194334800025	2.7827087002540694	9.2861208469999994	F	F	F
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6.2478796223200028	2.7827087002540694	10.5722416939999988	F	F	F
10.5949043483453682	4.1740630503811040	9.2861208469999994	F	F	F
11.2726743297746417	4.1740630503811040	12.5708101129999967	F	F	F
6.2478796223200028	2.7827087002540698	12.5708101129999967	F	F	F
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6.0839486494712522	2.7831097234319078	14.6359916440574924	T	T	T
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6.2478796223200028	5.5654174005081387	10.5722416939999988	F	F	F
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17.3467253884002304	1.3913192083896189	19.3021945275399283	T	T	T
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15.6196990558000053	2.7827087002540694	9.2861208469999994	F	F	F
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17.5205539520946409	6.9567717506351743	12.5708101129999967	F	F	F
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Metal reference: TiO2(110)/fcc(111)_7x3sqrt3/Rh E_tot= -895.65216216 eV
 D3-zero damping= -45.3882229 eV, D3-BJ damping= -54.7939555 eV
Rh
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     0.0000000000000009   13.9135435012703432    0.0000000000000000
     0.0000000000000000    0.0000000000000000   35.0099083997701825
 126
Cartesian
 17.7618240643330019  0.5440311728015290 22.9656802473280237
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Interface: TiO2(110)/fcc(111)_7x3sqrt3/Os E_tot= -4543.24507486 eV
 D3-zero damping= -113.384675164 eV, D3-BJ damping= -146.717272697 eV
Ti  O Os
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 120 240 126
Selective dynamics
Cartesian
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0.0000000000000006	0.0000000000000006	10.5722416939999970	F	F	F
4.3969480837233972	1.4073333438719398	9.2861208469999976	F	F	F
5.0825019070566073	1.4073333438719400	12.5708101129999950	F	F	F
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1.2371314201300629	1.4073333438719400	12.5708101129999950	F	F	F
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Oxide reference: TiO2(110)/fcc(111)_7x3sqrt3/Os E_tot= -3162.50295589 eV
 D3-zero damping= -54.2517243 eV, D3-BJ damping= -78.3829626 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
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    18.9588999815600054    0.0000000000000012    0.0000000000000000
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   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4
2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2
4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4
2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2
4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2
2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2
Selective dynamics
Cartesian
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  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
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3.1598166635933351	8.4440000632316377	11.2846892659999973	F	F	F
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4.3969480837233981	9.8513334071035779	9.2861208469999994	F	F	F
5.0825019070566082	9.8513334071035779	12.5708101129999967	F	F	F
0.0000000000000013	8.4440000632316377	12.5708101129999967	F	F	F
18.9603790750797998	9.8518216074403604	15.8578322544403214	T	T	T
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1.8999743213013287	9.8524277042082726	15.9870217945242725	T	T	T
3.1603953790564394	8.4443100299748881	16.2125137622835958	T	T	T
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5.1212038901482684	9.8525189142315881	19.5728068400698660	T	T	T
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3.1596761711520913	8.4456403288458564	20.7993419909437733	T	T	T
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0.0000000000000012	11.2586667509755127	8.0000000000000000	F	F	F
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10.7165814109100666	1.4073333438719398	9.2861208469999994	F	F	F
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7.5567647473167323	1.4073333438719400	12.5708101129999967	F	F	F
8.2193919833078937	1.4070592697712465	15.9844931557969971	T	T	T
9.4801041436962610	0.0004348806544934	16.2121175380966491	T	T	T
9.4790218896229952	1.4079919863582742	19.6362969288257254	T	T	T
9.4808027038491343	0.0022131151912770	18.0865915544558220	T	T	T
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11.4379997137595542	1.4093174413288538	19.5662969860924143	T	T	T
6.3202457541905659	0.0023791234236669	19.1203669277351764	T	T	T
9.4785604668616426	-0.0016688864874223	20.7999873191726259	T	T	T
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9.4794499907800027	4.2220000316158188	12.5708101129999967	F	F	F
9.4794499907800027	2.8146666877438791	11.2846892659999973	F	F	F
6.3196333271866694	2.8146666877438786	10.5722416939999988	F	F	F
10.7165814109100666	4.2220000316158188	9.2861208469999994	F	F	F
11.4021352342432767	4.2220000316158188	12.5708101129999967	F	F	F
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8.2191176443534069	4.2216430840759065	15.9826765012748933	T	T	T
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9.4724499350400642	5.6286718064937302	18.0881308808927912	T	T	T
6.3235740450581854	5.6298470417638837	17.2952836812830171	T	T	T
10.7400555563308586	7.0348883518849847	15.9870800635627734	T	T	T
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12.6392666543733370	5.6293333754877573	8.0000000000000000	F	F	F
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12.6392666543733370	5.6293333754877573	10.5722416939999988	F	F	F
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13.8763980745033972	7.0366667193596983	12.5708101129999967	F	F	F
14.5383883950528148	7.0364457185277463	15.9820843243760606	T	T	T
15.7976994934842434	5.6288892580059082	16.2125193320388874	T	T	T
15.7970891689481618	7.0385543249806801	19.6288303190340692	T	T	T
15.7914210709345610	5.6286991375986783	18.0867810376493168	T	T	T
12.6425699105311509	5.6296768727669226	17.2959849885420951	T	T	T
17.0603549311639640	7.0351669661486005	15.9884227679129385	T	T	T
17.7563886191542863	7.0388998830318785	19.5595922123345005	T	T	T
12.6377349363824170	5.6310065387362283	19.1218420919802554	T	T	T
15.8020217690103362	5.6325408567885535	20.7998533363341949	T	T	T
13.8371475640665142	7.0384336668238090	19.5728836165918914	T	T	T
12.6392666543733370	9.8513334071035779	9.2861208469999994	F	F	F
12.6392666543733370	8.4440000632316377	8.0000000000000000	F	F	F
14.5619518978366127	9.8513334071035779	9.2861208469999994	F	F	F
15.7990833179666712	8.4440000632316377	9.2861208469999994	F	F	F
15.7990833179666712	9.8513334071035779	12.5708101129999967	F	F	F
15.7990833179666712	8.4440000632316377	11.2846892659999973	F	F	F

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 17.0362147380967350  9.8513334071035779  9.2861208469999994   F   F   F
 17.7217685614299434  9.8513334071035779 12.5708101129999967   F   F   F
 12.6392666543733370  8.4440000632316377 12.5708101129999967   F   F   F
 12.6406801436525367  9.8514734244129016 15.8568868351057031   T   T   T
 12.6393588145264033  8.4431524146230323 14.6291381071161446   T   T   T
 15.7990833179666712  8.4440000632316377 13.8569309599999961   F   F   F
 13.8763980745033972  9.8513334071035779 12.5708101129999967   F   F   F
 14.5389529357931657  9.8523978643676315 15.9849501778979324   T   T   T
 15.7993236693685351  8.4435227639903072 16.2052078253129892   T   T   T
 15.8008449054243751  9.8524192254256420 19.6262352629290184   T   T   T
 15.7978099024738246  8.4441553691851379 18.0821722426926108   T   T   T
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 12.6394552130081816  8.4455487076024287 19.1201530687520176   T   T   T
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 13.8412669478993369  9.8533484697706566 19.5606486256206438   T   T   T
 12.6392666543733370 12.6660000948474547  9.2861208469999994   F   F   F
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 15.7990833179666712 11.2586667509755127 11.2846892659999973   F   F   F
 12.6392666543733370 11.2586667509755127 10.5722416939999988   F   F   F
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 17.7610060649108945 12.6676156129694331 19.5717654404107932   T   T   T
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 15.7979424907633081 11.2584523596201382 20.7963621270051391   T   T   T
 13.8417704947027644 12.6666405887618545 19.5625680356821086   T   T   T

Metal reference: TiO2(110)/fcc(111)_7x3sqrt3/Os E_tot= -1359.0103188 eV
 D3-zero damping= -44.8886417 eV, D3-BJ damping= -52.9036664 eV
Os
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    18.9588999815600054    0.0000000000000012    0.0000000000000000
     0.0000000000000009   14.0733334387193914    0.0000000000000000
     0.0000000000000000    0.0000000000000000   35.1342126897539089
 126
Cartesian
 18.0431641325971519  0.5667416845634582 22.8574405329707737
 16.6881463124978495  1.3507198557063587 25.0022963769997695
 18.0423524228268555  3.6953264792368108 25.0034192557426387
 18.0407509507109047  2.1327825136289231 27.1506182413620962
 16.6888535587401279  2.9127424663351773 22.8556409666257672
 16.6869524874065576  4.4784861617613840 27.1492779729422651
 15.3347817098518586  0.5680146252424316 22.8538381887949384
 13.9795855348381064  1.3507219482334387 24.9993252901466469
 15.3341062451489893  3.6964221095564227 25.0006823925080219
 15.3331760097979615  2.1341229850550576 27.1477917644969899
 13.9797006395397627  2.9141652763558956 22.8530385098176190
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12.6253617602712769	3.6969073849875875	24.9992760352325440
12.6254387686987553	2.1344891067825800	27.1459657620540469
11.2705315540516171	2.9143450111221281	22.8521632868288904
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9.9174597563135993	2.1346885570182002	27.1464175655432598
8.5622412106293027	2.9131697581240918	22.8538355566734417
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5.8545140515622940	1.3500268248099325	25.0039103315744278
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7.2100699975349611	2.1337067324294936	27.1490040494668818
5.8539896810707237	2.9120833787517304	22.8569773473547571
5.8556974008347815	4.4781603221194395	27.1503404039147753
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3.1461462473486721	1.3497243474097693	25.0064472419211796
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3.1464146494257710	2.9117828733887170	22.8585906700935588
3.1465565718816930	4.4780870330198308	27.1525623657029804
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0.4376697472860075	1.3495987726499357	25.0059425769595549
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18.0413666270031676	6.8238586895753750	27.1505956881742065
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9.9173228101807887	8.3873651933399849	25.0006775114556419
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  4.5006290792839314 11.5148776179616590 27.1517675336536506
  3.1461893710220545 12.2938264377090771 22.8587785028205026
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  1.7915902437741684  9.9481750505947861 22.8578609026518009
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  1.7919788113502013 13.0768980885597426 25.0053048091641621
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  0.4382706819221369 12.2937148982155993 22.8585412014065739
  0.4365351691883822 13.8603564221106339 27.1522093943253893

Interface: TiO2(110)/fcc(111)_7x3sqrt3/Ru E_tot= -4291.51507389 eV
 D3-zero damping= -119.675843864 eV, D3-BJ damping= -148.057144186 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
Ru
 1.0000000000000000
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     0.0000000000000008   13.8539542677392173    0.0000000000000000
     0.0000000000000000    0.0000000000000000   35.0551322736688604
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4
2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2
4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4
2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2   2
4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2   1   2
2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4   1   2 126
Selective dynamics
Cartesian
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  0.0000000000000005  0.0000000000000005  8.0000000000000018   F   F   F
  1.8927138726715942  1.3853954267739226  9.2861208470000012   F   F   F
  3.1105605322633343  0.0000000000000005  9.2861208470000012   F   F   F
  3.1105605322633343  1.3853954267739228 12.5708101129999985   F   F   F
  3.1105605322633343  0.0000000000000006 11.2846892659999991   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
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  3.1105605322633343  0.0000000000000008 13.8569309599999979   F   F   F
  1.2178466595917412  1.3853954267739228 12.5708101129999985   F   F   F
  1.9231800965136980  1.3284518788720177 15.9912769462954074   T   T   T
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  3.0513136969529944 -0.0984110898024464 18.2820974423276077   T   T   T
 18.7200373184234188 -0.0009868304011592 17.4522915041986160   T   T   T
  4.3804056405814986  1.3913515708831490 16.1343336446324805   T   T   T
  5.1938084491007865  1.3939702352188215 19.3948268247626849   T   T   T
  0.0705159992080302  0.1160091189203065 19.3008259843385019   T   T   T
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  1.2956743339991859  1.4353898738001616 19.8867151993780418   T   T   T
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  1.8927138726715944  4.1561862803217666  9.2861208470000012   F   F   F
  3.1105605322633343  2.7707908535478443  9.2861208470000012   F   F   F
  3.1105605322633343  4.1561862803217666 12.5708101129999985   F   F   F
  3.1105605322633343  2.7707908535478447 11.2846892659999991   F   F   F
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  0.0000000000000009  2.7707908535478447 12.5708101129999985   F   F   F
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  3.1105605322633343  2.7707908535478447 13.8569309599999979   F   F   F
  1.2178466595917414  4.1561862803217666 12.5708101129999985   F   F   F
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  3.2218783528366171  4.1099905782030426 19.5846558253774248   T   T   T
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12.4422421290533354	2.7707908535478443	10.5722416940000006	F	F	F
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13.6600887886450746	4.1561862803217666	12.5708101129999985	F	F	F
14.2704815286685402	4.2065854289290572	15.8748268349145398	T	T	T
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Oxide reference: TiO2(110)/fcc(111)_7x3sqrt3/Ru E_tot= -3137.02002603 eV
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O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
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Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
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Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
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Selective dynamics
Cartesian
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Metal reference: TiO2(110)/fcc(111)_7x3sqrt3/Ru E_tot= -1121.8940451 eV
 D3-zero damping= -43.3316443 eV, D3-BJ damping= -52.7256435 eV
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Cartesian
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12.3353589176907583	9.7155860766232571	22.9566199217431617
11.0035252211614800	10.4851807234961889	25.0680983790318841
12.3359284728445644	12.7948673966666107	25.0715336354901410
12.3385201895543286	11.2585073113206633	27.1795181118653701
11.0023892390671048	12.0250631431745969	22.9570548870291731
11.0068736164869811	13.5623311720190554	27.1839599816307036
9.6688797685482530	9.7151314723420938	22.9562074539007384
8.3377669808871495	10.4854336264539878	25.0652839390496851
9.6696646730286204	12.7943546803956956	25.0689543093653029
9.6698384435943652	11.2543183917348575	27.1812160008803616
8.3396720805469045	12.0233620977213196	22.9553805304125049
8.3378130600822598	13.5637026834811927	27.1785687037224548
7.0069510521161966	9.7168669626803190	22.9517992731307316
5.6717655562566529	10.4865318107627097	25.0623997331566244
7.0055175213168086	12.7938614665457973	25.0658251665875547
7.0043756801259516	11.2549494583730620	27.1776836251029366
5.6717778306304263	12.0259946235141282	22.9540667329962069
5.6705414783518551	13.5651525961315915	27.1763692741984819
4.3423964132315520	9.7176847816484706	22.9519954203985144
3.0055252421692091	10.4859173433671344	25.0629424427284953

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  1.6722926698422929  9.7162269968448616 22.9530253088840439
  0.3373583979740396 10.4870577366665074 25.0622611363664411
  1.6716100901621775 12.7957151422381070 25.0701600181004167
  1.6686910034597349 11.2588821333891058 27.1765522877614352
  0.3383376701530920 12.0269782982164255 22.9541259740801991
  0.3412414622666357 13.5673201115057314 27.1776225887036809

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt13/Au E_tot= -1145.76589388 eV
 D3-zero damping= -37.217341 eV, D3-BJ damping= -44.0470219 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Au
 1.0000000000000000
    10.4515979269385308    0.0000000000000000    0.0000000000000000
    -5.2257989634692636    9.0513493148695456    0.0000000000000000
     0.0000000000000022    0.0000000000000039   36.5299760590939258
  11  18   1   3   3  11  18   1   3   3  11  18   1   3   3  11  18   1
3   3  39
Selective dynamics
Cartesian
  0.0257131673562849 -0.0650841224619635 12.3918657751636410   F   F   F
  2.6471498001012921  1.4464523705508714 16.6956885131836792   T   T   T
  0.0199257717797911 -0.0543655083943579 18.7849247570011606   T   T   T
  2.6409249752535868  1.4434144694982136 10.0985295441362908   F   F   F
  0.0256151480453494  2.9547041618686904 14.5561856244294319   F   F   F
  0.0622203337368628 -0.0498162537516603  9.7781175373791633   F   F   F
  2.6396181753482013  1.4467419585392116 14.0665571956713542   F   F   F
  0.0313106005212093  2.9303371686098876 18.1226775392104074   T   T   T
  0.0278195537191837 -0.0636261219396585 16.0914179558055004   T   T   T
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  0.0317554923648654  2.9536172403588399 11.8834768182986394   F   F   F
  1.6484949300699963 -0.0605833488553652 11.0348070799988349   F   F   F
  4.2139137653795542  1.4524250646949679 15.3495719264051740   T   T   T
  1.6233168054858285  2.9797396071523994 19.5210318117082267   T   T   T
  0.8202457373859596  1.3013642134150372 17.4052382757925876   T   T   T
  3.4409374496916594  2.8964268355175693  8.8712015584813955   F   F   F
  0.8286764729630932  4.3413851500938510 13.2250185171475501   F   F   F
 -0.7853800668616548  1.3360232616171857 11.0371856277262985   F   F   F
  1.8461326200990882  2.8092526694794060 15.3430869702839701   T   T   T
 -0.8277630478942805  4.3496766390390711 19.4985668041207774   T   T   T
  3.6711372497600978 -0.0717131338753856 17.4303380971845385   T   T   T
  1.0200145689575191  1.3858908143526665  8.8494658732768272   F   F   F
 -1.5740045769364852  2.9565004788367499 13.2250148374957810   F   F   F
  1.8456928478687222  3.0659563383269877 11.0407582029264013   F   F   F
  1.8603587884982669  0.0730480682853381 15.3412515964961411   T   T   T
 -0.7230534511773687  1.5792598384449366 19.4868905581754888   T   T   T
 -1.7978501238763869  3.0979139345936546 17.4228165353192139   T   T   T
  3.5153508056762082 -0.0003321130180469  8.9135372731794220   F   F   F
  0.8273080294502347  1.5652636205319386 13.2221143204608858   F   F   F
 -0.0790022611568277  2.9277464817297014 20.7032197886447911   T   T   T
  3.6000319872043174  2.7718784635882714 21.5536064820078010   T   T   T
  1.0553291635560660  1.7647462872335746 21.6041194057391124   T   T   T
  3.1915823435125268  0.0442959529947772 21.5839883656770830   T   T   T
  0.4568637393702998  2.3012763227880537  8.8276013437729759   F   F   F
  2.9145005330463536  2.7487503723783631  8.0391937587954843   F   F   F
  3.4466711905434533  0.3394291636635692  8.0000000000000000   F   F   F
 -2.5871863143783469  4.4605905349728099 12.3918657751636410   F   F   F
  0.0227013930164188  5.9762487632663079 16.6983028968046483   T   T   T
 -2.6290782641690740  4.4535697358569006 18.8076157536900830   T   T   T
  0.0280254935189548  5.9690891269329862 10.0985295441362908   F   F   F
 -2.5872843336892828  7.4803788193034642 14.5561856244294319   F   F   F
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-2.5506791479977688	4.4758584036831124	9.7781175373791633	F	F	F
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-2.6084664678294169	7.4921520004849578	18.1345733036103134	T	T	T
-2.5838588336361492	4.4635879203929800	16.1101440421008881	T	T	T
-0.0171717864819253	5.9888089398415527	20.3891986906236014	T	T	T
-2.5811439893697665	7.4792918977936127	11.8834768182986394	F	F	F
-0.9644045516646357	4.4650913085794075	11.0348070799988349	F	F	F
1.6021603060262903	5.9783852366505901	15.3484042282228526	T	T	T
-0.9685770013290851	7.5112993170717317	19.5443021031726083	T	T	T
-1.8068839715642242	5.8548263206100764	17.4316242997135049	T	T	T
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-1.7842230087715387	8.8670598075286229	13.2250185171475501	F	F	F
-3.3982795485962871	5.8616979190519585	11.0371856277262985	F	F	F
-0.7609142453665939	7.3338784064223317	15.3480978641868671	T	T	T
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-1.5928849127771130	5.9115654717874389	8.8494658732768272	F	F	F
-4.1869040586711170	7.4821751362715219	13.2250148374957810	F	F	F
-0.7672066338659097	7.5916309957617614	11.0407582029264013	F	F	F
-0.7574020369452382	4.6074138992634968	15.3484724880691026	T	T	T
-3.3622546944258449	6.0987290064189672	19.5582693144693636	T	T	T
-4.4164262645271526	7.6171540724814113	17.4231862770298953	T	T	T
0.9024513239415760	4.5253425444167261	8.9135372731794220	F	F	F
-1.7855914522843974	6.0909382779667114	13.2221143204608858	F	F	F
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-1.4762839119513969	6.3744881406257532	21.6635093455760988	T	T	T
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-2.1560357423643324	6.8269509802228256	8.8276013437729759	F	F	F
0.3016010513117213	7.2744250298131359	8.0391937587954843	F	F	F
0.8337717088088210	4.8651038210983417	8.0000000000000000	F	F	F
5.2515121308255504	-0.0650841224619635	12.3918657751636410	F	F	F
7.8575922569044918	1.4442540004280717	16.7028367528683646	T	T	T
5.2499964709500961	-0.0376054753615567	18.8047645614008268	T	T	T
7.8667239387228536	1.4434144694982136	10.0985295441362908	F	F	F
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5.2880192972061284	-0.0498162537516603	9.7781175373791633	F	F	F
7.8654171388174676	1.4467419585392116	14.0665571956713542	F	F	F
5.2425174937907144	2.9529723965135699	18.1745184586113204	T	T	T
5.2552141945713675	-0.0630507694396684	16.1090778171651756	T	T	T
7.7399364522786174	1.4411030890203123	20.5686783344890749	T	T	T
5.2575544558341321	2.9536172403588399	11.8834768182986394	F	F	F
6.8742938935392619	-0.0605833488553652	11.0348070799988349	F	F	F
9.4406847508626583	1.4514382105589700	15.3432486483383421	T	T	T
6.8114577074327958	2.9505848101023076	19.5241557241722603	T	T	T
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4.4404188966076106	1.3360232616171857	11.0371856277262985	F	F	F
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4.4551777124668464	4.3457959976229628	19.5151044629884183	T	T	T
8.8848848811822290	-0.0643312443214065	17.4287588859008586	T	T	T
6.2458135324267854	1.3858908143526665	8.8494658732768272	F	F	F
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7.0714918113379879	3.0659563383269877	11.0407582029264013	F	F	F
7.0794546286154354	0.0792679537316202	15.3457036517672272	T	T	T
4.4376671444027780	1.5856344071203496	19.5067096335033909	T	T	T
3.4305714090021486	3.1046676025095929	17.4265445728944961	T	T	T
8.7411497691454727	-0.0003321130180469	8.9135372731794220	F	F	F
6.0531069929195018	1.5652636205319386	13.2221143204608858	F	F	F
5.2424788554984287	2.9816717040587073	20.7669751113656247	T	T	T
8.7750478289844764	2.6472171877132089	21.5625216649963036	T	T	T
6.1997253321769561	1.6498405156072702	21.6126985931066535	T	T	T

8.4309810683445914	-0.0500278027663507	21.6859089631178747	T	T	T
5.6826627028395649	2.3012763227880537	8.8276013437729759	F	F	F
8.1402994965156186	2.7487503723783631	8.0391937587954843	F	F	F
8.6724701540127196	0.3394291636635692	8.0000000000000000	F	F	F
2.6386126490909194	4.4605905349728099	12.3918657751636410	F	F	F
5.2517466492947662	5.9661690723691878	16.6986350823302629	T	T	T
2.6535485246708719	4.4670214031204871	18.8062310382363940	T	T	T
5.2538244569882213	5.9690891269329862	10.0985295441362908	F	F	F
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2.6751198154714970	4.4758584036831124	9.7781175373791633	F	F	F
5.2525176570828354	5.9724166159739855	14.0665571956713542	F	F	F
2.6531542710616045	7.4720623667284638	18.1430671902696155	T	T	T
2.6379330341042193	4.4625333360241548	16.1084598752232147	T	T	T
5.2932704255779104	5.9368316755468094	20.5446444925825489	T	T	T
2.6446549740994998	7.4792918977936127	11.8834768182986394	F	F	F
4.2613944118046305	4.4650913085794075	11.0348070799988349	F	F	F
6.8272374071401076	5.9760173796785310	15.3460830584008345	T	T	T
4.2130164897020128	7.5284856740278734	19.5216571977543971	T	T	T
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6.0538369314262930	7.4221014929523417	8.8712015584813955	F	F	F
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1.8275194148729792	5.8616979190519585	11.0371856277262985	F	F	F
4.4560774297450152	7.3349014034550750	15.3425294116528601	T	T	T
1.7992267936420525	8.8658993899781322	19.6036429372668053	T	T	T
6.2929733756284092	4.4628250734322785	17.4423720434798710	T	T	T
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4.4585923296033574	7.5916309957617614	11.0407582029264013	F	F	F
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3.4402075111848687	6.0909382779667114	13.2221143204608858	F	F	F
2.6964582435703668	7.4824529805357463	20.7404425952020297	T	T	T
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0.9004116977222473	2.6563266325951944	23.7739984800124553	T	T	T
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4.0558461226443061	6.1214374731614676	23.6751586913708607	T	T	T
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2.7760165154314160	8.6357222915963767	23.7977076792993820	T	T	T
9.2713618625158674	0.9905916420172721	25.9251233203627329	T	T	T
1.7117993897336419	1.3041702299993829	26.0436700057212605	T	T	T
7.1714116410834476	3.0360558096152115	25.9788903005841121	T	T	T
-0.5291855400540479	3.9340717860267502	25.8197169597944871	T	T	T
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0.5088520888829607	6.5157026230637545	25.1241206393958443	T	T	T
3.0704405369823227	7.0621962286516293	26.0948258944136633	T	T	T
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0.0604326709270834	2.1830150098678178	28.2180156427470656	T	T	T
2.8482662266809746	2.8302241746154935	28.3668886112466829	T	T	T
8.4832338050669236	4.2327519989766076	28.3722718715120052	T	T	T
0.8519086306478714	4.9589520193874348	28.2152428432537832	T	T	T

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  3.6459270331147673  5.6067214993877155 28.5134278694267742   T   T   T
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 -3.7687665067747571  6.9747904985825491 23.7043241202911048   T   T   T
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  5.8077352387350594  7.8101007508597524 26.1135966325992541   T   T   T
  4.8359678086808691  0.7079480587343547 28.4695038375718426   T   T   T
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Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Au E_tot= -1067.5475268 eV
 D3-zero damping= -15.2104243 eV, D3-BJ damping= -22.8738703 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H
 1.0000000000000000
    10.4515979269385308    0.0000000000000000    0.0000000000000000
    -5.2257989634692636    9.0513493148695456    0.0000000000000000
     0.0000000000000019    0.0000000000000032   30.5466344559568874
  11  18   1   3   6  11  18   1   3   6  11  18   1   3   6  11  18   1
3   6
Selective dynamics
Cartesian
  0.0257131673562849 -0.0650841224619635 12.3918657751636392   F   F   F
  2.6397485400689060  1.4435069609737554 16.6998779244377928   T   T   T
  0.0207475062714569 -0.0699810787876196 18.7822530369640042   T   T   T
  2.6409249752535868  1.4434144694982136 10.0985295441362890   F   F   F
  0.0256151480453494  2.9547041618686904 14.5561856244294301   F   F   F
  0.0622203337368628 -0.0498162537516603  9.7781175373791616   F   F   F
  2.6396181753482013  1.4467419585392116 14.0665571956713524   F   F   F
  0.0304932748022114  2.9504991997399035 18.1642674679613521   T   T   T
  0.0261152108377820 -0.0628075102926868 16.1010647170171168   T   T   T
  2.6355116141016417  1.4230540503942788 20.4531223139616465   T   T   T
  0.0317554923648654  2.9536172403588399 11.8834768182986377   F   F   F
  1.6484949300699963 -0.0605833488553652 11.0348070799988349   F   F   F
  4.2148517447623730  1.4519112878513609 15.3487720785794330   T   T   T
  1.6102783909808389  2.9761156679537093 19.5464441202584176   T   T   T
  0.8115139365390397  1.3042462637489771 17.4376721063581108   T   T   T
  3.4409374496916594  2.8964268355175693  8.8712015584813955   F   F   F
  0.8286764729630932  4.3413851500938510 13.2250185171475483   F   F   F
 -0.7853800668616548  1.3360232616171857 11.0371856277262967   F   F   F
  1.8470885800108803  2.8053635526508875 15.3484762407148736   T   T   T
 -0.7841560097637166  4.3246633046404881 19.5488888535930663   T   T   T
  3.6722745073828329 -0.0698455868565824 17.4331226189141084   T   T   T
  1.0200145689575191  1.3858908143526665  8.8494658732768272   F   F   F
 -1.5740045769364852  2.9565004788367499 13.2250148374957792   F   F   F
  1.8456928478687222  3.0659563383269877 11.0407582029264013   F   F   F
  1.8565913995810572  0.0783472755134891 15.3494648655574082   T   T   T
 -0.7629118243653790  1.5504234729599506 19.5501338459762870   T   T   T
 -1.7933970824942407  3.0945260792735385 17.4404152700765493   T   T   T
  3.5153508056762082 -0.0003321130180469  8.9135372731794220   F   F   F
  0.8273080294502347  1.5652636205319386 13.2221143204608840   F   F   F
  0.0192421304673816  2.9453060979141661 20.7677655247032078   T   T   T
  3.6031408259640916  2.6206991764575305 21.6263370229995822   T   T   T
  1.0769711672564948  1.6537504466224628 21.6339079573244746   T   T   T
  3.2824016901765249 -0.0454200467648080 21.6254423641440958   T   T   T
  0.5296568274525902  0.8659855051518720 21.7939822834615171   T   T   T
  3.0367256217252705  3.2671292115712411 22.0750056602187854   T   T   T
```

3.0586718009252900	0.1617953635453346	22.5465772273854554	T	T	T
0.4568637393702998	2.3012763227880537	8.8276013437729759	F	F	F
2.9145005330463536	2.7487503723783631	8.0391937587954807	F	F	F
3.4466711905434533	0.3394291636635692	8.0000000000000000	F	F	F
-2.5871863143783469	4.4605905349728090	12.3918657751636392	F	F	F
0.0268490583342740	5.9691816184085287	16.6998779244377928	T	T	T
-2.5921519754631750	4.4556935786471534	18.7822530369640042	T	T	T
0.0280254935189550	5.9690891269329862	10.0985295441362890	F	F	F
-2.5872843336892823	7.4803788193034633	14.5561856244294301	F	F	F
-2.5506791479977688	4.4758584036831124	9.7781175373791616	F	F	F
0.0267186936135695	5.9724166159739847	14.0665571956713524	F	F	F
-2.5824062069324203	7.4761738571746772	18.1642674679613521	T	T	T
-2.5867842708968500	4.4628671471420853	16.1010647170171168	T	T	T
0.0226121323670100	5.9487287078290514	20.4531223139616465	T	T	T
-2.5811439893697665	7.4792918977936127	11.8834768182986377	F	F	F
-0.9644045516646356	4.4650913085794075	11.0348070799988349	F	F	F
1.6019522630277410	5.9775859452861342	15.3487720785794330	T	T	T
-1.0026210764680787	7.5017903253884821	19.5464441202584176	T	T	T
-1.8013855451955920	5.8299209211837502	17.4376721063581108	T	T	T
0.8280379679570276	7.4221014929523417	8.8712015584813955	F	F	F
-1.7842230087715385	8.8670598075286229	13.2250185171475483	F	F	F
-3.3982795485962867	5.8616979190519585	11.0371856277262967	F	F	F
-0.7658109017237514	7.3310382100856604	15.3484762407148736	T	T	T
-3.3970554914983482	8.8503379620752600	19.5488888535930663	T	T	T
1.0593750256482009	4.4558290705781900	17.4331226046283945	T	T	T
-1.5928849127771127	5.9115654717874389	8.8494658732768272	F	F	F
-4.1869040586711170	7.4821751362715228	13.2250148374957792	F	F	F
-0.7672066338659096	7.5916309957617605	11.0407582029264013	F	F	F
-0.7563080821535746	4.6040219329482621	15.3494648655574082	T	T	T
-3.3758113061000108	6.0760981303947235	19.5501338459762870	T	T	T
-4.4062965642288727	7.6202007367083118	17.4404152700765493	T	T	T
0.9024513239415763	4.5253425444167261	8.9135372731794220	F	F	F
-1.7855914522843972	6.0909382779667114	13.2221143204608840	F	F	F
-2.5936573512672503	7.4709807553489389	20.7677655247032078	T	T	T
0.9902413585151740	7.1463738338923033	21.6263370229995822	T	T	T
-1.5359283144781370	6.1794251040572359	21.6339079573244746	T	T	T
0.6695022084418929	4.4802546106699648	21.6254423784298098	T	T	T
-2.0832426542820417	5.3916601625866454	21.7939822834615171	T	T	T
0.4238261399906385	7.7928038690060140	22.0750056602187854	T	T	T
0.4457723191906580	4.6874700209801068	22.5465772273854554	T	T	T
-2.1560357423643319	6.8269509802228265	8.8276013437729759	F	F	F
0.3016010513117218	7.2744250298131359	8.0391937587954807	F	F	F
0.8337717088088215	4.8651038210983417	8.0000000000000000	F	F	F
5.2515121308255504	-0.0650841224619635	12.3918657751636392	F	F	F
7.8655475035381706	1.4435069609737554	16.6998779244377928	T	T	T
5.2465464697407231	-0.0699810787876196	18.7822530369640042	T	T	T
7.8667239387228527	1.4434144694982136	10.0985295441362890	F	F	F
5.2514141115146149	2.9547041618686904	14.5561856244294301	F	F	F
5.2880192972061284	-0.0498162537516603	9.7781175373791616	F	F	F
7.8654171388174667	1.4467419585392116	14.0665571956713524	F	F	F
5.2562922382714765	2.9504991997399035	18.1642674679613521	T	T	T
5.2519141743070472	-0.0628075102926868	16.1010647170171168	T	T	T
7.8613105775709071	1.4230540503942788	20.4531223139616465	T	T	T
5.2575544558341312	2.9536172403588399	11.8834768182986377	F	F	F
6.8742938935392619	-0.0605833488553652	11.0348070799988349	F	F	F
9.4406507082316384	1.4519112878513609	15.3487720785794330	T	T	T
6.8360773544501043	2.9761156679537093	19.5464441202584176	T	T	T
6.0373129000083052	1.3042462637489771	17.4376721063581108	T	T	T
8.6667364131609244	2.8964268355175693	8.8712015584813955	F	F	F
6.0544754364323587	4.3413851500938510	13.2250185171475483	F	F	F
4.4404188966076106	1.3360232616171857	11.0371856277262967	F	F	F
7.0728875434801459	2.8053635526508875	15.3484762407148736	T	T	T
4.4416429537055482	4.3246633046404881	19.5488888535930663	T	T	T

8.8980734708520988	-0.0698455868565824	17.4331226189141084	T	T	T
6.2458135324267845	1.3858908143526665	8.8494658732768272	F	F	F
3.6517943865327802	2.9565004788367499	13.2250148374957792	F	F	F
7.0714918113379879	3.0659563383269877	11.0407582029264013	F	F	F
7.0823903630503224	0.0783472755134891	15.3494648655574082	T	T	T
4.4628871391038869	1.5504234729599506	19.5501338459762870	T	T	T
3.4324018809750245	3.0945260792735385	17.4404152700765493	T	T	T
8.7411497691454727	-0.0003321130180469	8.9135372731794220	F	F	F
6.0531069929195001	1.5652636205319386	13.2221143204608840	F	F	F
5.2450410939366474	2.9453060979141661	20.7677655247032078	T	T	T
8.8289397894333561	2.6206991764575305	21.6263370229995822	T	T	T
6.3027701307257606	1.6537504466224628	21.6339079573244746	T	T	T
8.5082006536457904	-0.0454200467648080	21.6254423784298098	T	T	T
5.7554557909218564	0.8659855051518720	21.7939822834615171	T	T	T
8.2625245851945373	3.2671292115712411	22.0750056602187854	T	T	T
8.2844707643945554	0.1617953635453346	22.5465772273854554	T	T	T
5.6826627028395649	2.3012763227880537	8.8276013437729759	F	F	F
8.1402994965156186	2.7487503723783631	8.0391937587954807	F	F	F
8.6724701540127178	0.3394291636635692	8.0000000000000000	F	F	F
2.6386126490909185	4.4605905349728090	12.3918657751636392	F	F	F
5.2526480218035392	5.9691816184085287	16.6998779244377928	T	T	T
2.6336469880060904	4.4556935786471534	18.7822530369640042	T	T	T
5.2538244569882204	5.9690891269329862	10.0985295441362890	F	F	F
2.6385146297799831	7.4803788193034633	14.5561856244294301	F	F	F
2.6751198154714966	4.4758584036831124	9.7781175373791616	F	F	F
5.2525176570828354	5.9724166159739847	14.0665571956713524	F	F	F
2.6433927565368451	7.4761738571746772	18.1642674679613521	T	T	T
2.6390146925724154	4.4628671471420853	16.1010647170171168	T	T	T
5.2484110958362757	5.9487287078290514	20.4531223139616465	T	T	T
2.6446549740994989	7.4792918977936127	11.8834768182986377	F	F	F
4.2613944118046296	4.4650913085794075	11.0348070799988349	F	F	F
6.8277512264970071	5.9775859452861342	15.3487720785794330	T	T	T
4.2231778870011869	7.5017903253884821	19.5464441202584176	T	T	T
3.4244134182736730	5.8299209211837502	17.4376721063581108	T	T	T
6.0538369314262930	7.4221014929523417	8.8712015584813955	F	F	F
3.4415759546977269	8.8670598075286229	13.2250185171475483	F	F	F
1.8275194148729788	5.8616979190519585	11.0371856277262967	F	F	F
4.4599880617455137	7.3310382100856604	15.3484762407148736	T	T	T
1.8287434719709170	8.8503379620752600	19.5488888535930663	T	T	T
6.2851739891174665	4.4558290705781900	17.4331226189141084	T	T	T
3.6329140506921527	5.9115654717874389	8.8494658732768272	F	F	F
1.0388949047981484	7.4821751362715228	13.2250148374957792	F	F	F
4.4585923296033556	7.5916309957617605	11.0407582029264013	F	F	F
4.4694908813156902	4.6040219329482621	15.3494648655574082	T	T	T
1.8499876573692546	6.0760981303947235	19.5501338459762870	T	T	T
0.8195023992403928	7.6202007367083118	17.4404152700765493	T	T	T
6.1282502874108413	4.5253425444167261	8.9135372731794220	F	F	F
3.4402075111848682	6.0909382779667114	13.2221143204608840	F	F	F
2.6321416122020151	7.4709807553489389	20.7677655247032078	T	T	T
6.2160403076987256	7.1463738338923033	21.6263370229995822	T	T	T
3.6898706489911284	6.1794251040572359	21.6339079573244746	T	T	T
5.8953011719111581	4.4802546106699648	21.6254423784298098	T	T	T
3.1425563091872237	5.3916601625866454	21.7939822834615171	T	T	T
5.6496251034599032	7.7928038690060140	22.0750056602187854	T	T	T
5.6715712826599232	4.6874700209801068	22.5465772273854554	T	T	T
3.0697632211049335	6.8269509802228265	8.8276013437729759	F	F	F
5.5274000147809872	7.2744250298131359	8.0391937587954807	F	F	F
6.0595706722780864	4.8651038210983417	8.0000000000000000	F	F	F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Au E_tot= -134.45156351 eV
 D3-zero damping= -16.876087 eV, D3-BJ damping= -17.2990027 eV
Au
 1.0000000000000000

```
    10.4515979269385308    0.0000000000000000    0.0000000000000000
    -5.2257989634692628    9.0513493148695439    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000676436712382  0.0000262980167339  7.8595086384984993
  2.8138849800795245  0.6978029952216056  7.8587478611780330
  8.4404065115875273  2.0880242030657707  7.8588050378192467
  0.8030089517970711  2.7856375619618721  7.8587901869474672
  3.6184955259381160  3.4808666731628848  7.8571738965841966
 -1.2054727274809207  4.8740931166142563  7.8591193484922108
  1.6075052966354850  5.5704141948994526  7.8591687135558166
  4.4232040535151498  6.2656128872572729  7.8587807553999207
 -0.4019242656636173  7.6583220908782481  7.8590825188619267
  2.4120383436496011  8.3540525555722915  7.8587895664942291
  8.8445039162870867  0.4647968941776787 10.2755520864748000
  1.2063226009228931  1.1593650275684138 10.2755837754173047
  6.8329809483950861  2.5537984134984182 10.2740842034512951
 -0.8020720513989207  3.2481349076053885 10.2750322900062816
  2.0116191117973359  3.9466580717831454 10.2741042582928745
  0.0000248879312608  6.0342429676442970 10.2740922232280116
  2.8139995857314988  6.7326567697732100 10.2750272999893362
  0.8021774807534926  8.8200899111924222 10.2740493675852811
 -3.6188345293885122  8.5863811881476000 12.6917955534697704
 -0.4006763176303467  1.6241122117887199 12.6918090122397853
  2.4128925697573109  2.3195217483836097 12.6906455539266236
  8.0402852802117337  3.7149694803866269 12.6901777835426568
  0.4027327597189356  4.4101647890427484 12.6904161343126347
  3.2142750878443667  5.1055579469870169 12.6902132084695189
 -1.6077677589304107  6.4974974552552647 12.6903966286473029
  1.2051982775833403  7.1949139773281612 12.6904219638344316
  4.0197617263688743  7.8922620508161572 12.6917823326009120
  7.2365291587633882  0.9296977153726051 12.6907325797777286
  5.6277923887529209  1.3932491412625354  7.8571225132595108
  6.4311102287952311  4.1771590027975964  7.8571674741332638
 -3.2148414737077249  6.9631804427554327  7.8587078568890183
 -2.0116813315394735  8.1219295943505312 10.2749759042997422
  4.0210524924150999  1.8568440441747116 10.2740789790561742
  4.8234102686626601  4.6405655624466551 10.2740810593326000
 -2.8136990261133432  5.3358516291346945 10.2741178146610803
  5.6267576264006030  7.4270248849843430 10.2755416321589372
  4.4230188736205900  0.2307521563163879 12.6901477739640463
  5.2259029450914527  3.0170448910076515 12.6906470746538069
  6.0280192813622273  5.8020892232561501 12.6906654145006303

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt13/Ag E_tot= -1127.44439888 eV
 D3-zero damping= -32.4511729 eV, D3-BJ damping= -42.984004 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Ag
 1.0000000000000000
    10.3858879861668498    0.0000000000000000    0.0000000000000000
    -5.1929439930834231    8.9944428368800988    0.0000000000000000
     0.0000000000000022    0.0000000000000038   36.2595747862226716
  11  18   1   3   3  11  18   1   3   3  11  18   1   3   3  11  18   1
3   3  39
Selective dynamics
Cartesian
  0.0255515068412283 -0.0646749339472456 12.3918657751636410   F   F   F
  2.6229758075120140  1.4438335901003996 16.6994165451957208   T   T   T
  0.0052795322718664 -0.0598136530001085 18.7989610676844201   T   T   T
  2.6243212917862877  1.4343396198950489 10.0985295441362908   F   F   F
  0.0254541037846838  2.9361277263005165 14.5561856244294319   F   F   F
  0.0618291500658850 -0.0495030554152555  9.7781175373791633   F   F   F
  2.6230227078250077  1.4376461887753853 14.0665571956713542   F   F   F
```

0.0229898740985784	2.9223498765377967	18.1548481204841963	T	T	T
0.0274098635964330	-0.0583475975354687	16.1065951330683035	T	T	T
2.6070919922621334	1.4298040258763156	20.5017084817575110	T	T	T
0.0315558433220054	2.9350476383436339	11.8834768182986394	F	F	F
1.6381307250006336	-0.0602024570249614	11.0348070799988349	F	F	F
4.1892338187773435	1.4436083373685706	15.3474012444497241	T	T	T
1.5995359741327884	2.9662544573880090	19.5405649555869516	T	T	T
0.8116511179276700	1.3014639120599618	17.4262756522954021	T	T	T
3.4193040308021394	2.8782167936520264	8.8712015584813955	F	F	F
0.8234665249400314	4.3140905523611490	13.2250185171475501	F	F	F
-0.7804423264283261	1.3276235881888594	11.0371856277262985	F	F	F
1.8320331402782770	2.7931762277640542	15.3446230089546063	T	T	T
-0.7849659493404331	4.3452898977333971	19.5425571136464704	T	T	T
3.6373522472671760	-0.0624010467970026	17.4344100876299706	T	T	T
1.0136016646934070	1.3771776200675696	8.8494658732768272	F	F	F
-1.5641086980242020	2.9379127496958226	13.2250148374957810	F	F	F
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Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Ag E_tot= -1070.80608321
eV
 D3-zero damping= -15.4305057 eV, D3-BJ damping= -23.1461124 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H
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3   6
Selective dynamics
Cartesian
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-1.7880798504659241	5.7965302555228515	17.4472636957184406	T	T	T
0.8228320342604278	7.3754382120920763	8.8712015584813955	F	F	F
-1.7730054716016803	8.8113119708011993	13.2250185171475483	F	F	F
-3.3769143229700376	5.8248450066289088	11.0371856277262967	F	F	F
-0.7614928745364757	7.2881334112136216	15.3518763069199267	T	T	T
-3.3735045635973591	8.7975076332755666	19.5622069309588937	T	T	T
1.0519225122214919	4.4295911424356218	17.4429044055532785	T	T	T
-1.5828703318483046	5.8743990385076188	8.8494658732768272	F	F	F
-4.1605806945659136	7.4351341681358720	13.2250148374957792	F	F	F
-0.7623831511005583	7.5439018708395116	11.0407582029264013	F	F	F

-0.7526862977517472	4.5742834896750617	15.3527726600999941	T	T	T
-3.3569946163549389	6.0392226319948659	19.5630469902082993	T	T	T
-4.3776254745774681	7.5729249735177158	17.4493383247139029	T	T	T
0.8967775481744580	4.4968913934402082	8.9135372731794220	F	F	F
-1.7743653116126810	6.0526441150753536	13.2221143204608840	F	F	F
-2.5767176810349133	7.4248149947544375	20.7855954725415906	T	T	T
0.9780375839593632	7.1111427571767400	21.6463547336711812	T	T	T
-1.5320234214062713	6.1288941069508835	21.6530296667340458	T	T	T
0.6832192627214635	4.4530191403349360	21.6447137680858859	T	T	T
-2.0882993602083086	5.3456357726009340	21.8052231538307240	T	T	T
0.4033177192371791	7.7606969270958741	22.0798017275417777	T	T	T
0.4344865457436733	4.6671484777370935	22.5581397871280025	T	T	T
-2.1424805920492562	6.7840294530365028	8.8276013437729759	F	F	F
0.2997048640151081	7.2286902013975656	8.0391937587954807	F	F	F
0.8285297266749962	4.8345165667696541	8.0000000000000000	F	F	F
5.2184954999246536	-0.0646749339472456	12.3918657751636392	F	F	F
7.8164915898315677	1.4364380397722893	16.7027816012770600	T	T	T
5.2146704090777156	-0.0680327836258789	18.7909959029545099	T	T	T
7.8172652848697126	1.4343396198950489	10.0985295441362890	F	F	F
5.2183980968681087	2.9361277263005165	14.5561856244294301	F	F	F
5.2547731431493103	-0.0495030554152555	9.7781175373791616	F	F	F
7.8159667009084330	1.4376461887753853	14.0665571956713524	F	F	F
5.2231781779378288	2.9340137298111588	18.1807575303043016	T	T	T
5.2194915799239725	-0.0610719983087398	16.1094975642247853	T	T	T
7.8125388640767293	1.4159032784322263	20.4659241119621029	T	T	T
5.2244998364054300	2.9350476383436339	11.8834768182986377	F	F	F
6.8310747180840590	-0.0602024570249614	11.0348070799988349	F	F	F
9.3841722645959429	1.4434540481541041	15.3525199088156761	T	T	T
6.7967551617468951	2.9554367373503565	19.5619103478012448	T	T	T
6.0013361391592133	1.2993088370828021	17.4472636957184406	T	T	T
8.6122480238855648	2.8782167936520264	8.8712015584813955	F	F	F
6.0164105180234566	4.3140905523611490	13.2250185171475483	F	F	F
4.4125016666550989	1.3276235881888594	11.0371856277262967	F	F	F
7.0279231150886607	2.7909119927735722	15.3518763069199267	T	T	T
4.4159114260277770	4.3002862148355181	19.5622069309588937	T	T	T
8.8413385018466286	-0.0676302760044280	17.4429044198389924	T	T	T
6.2065456577768323	1.3771776200675696	8.8494658732768272	F	F	F
3.6288352950592229	2.9379127496958226	13.2250148374957792	F	F	F
7.0270328385245779	3.0466804523994622	11.0407582029264013	F	F	F
7.0367296918733890	0.0770620712350116	15.3527726600999941	T	T	T
4.4324213732701976	1.5420012135548165	19.5630469902082993	T	T	T
3.4117905150476679	3.0757035550776664	17.4493383247139029	T	T	T
8.6861935377995945	-0.0003300249998417	8.9135372731794220	F	F	F
6.0150506780124555	1.5554226966353044	13.2221143204608840	F	F	F
5.2126983085902241	2.9275935763143881	20.7855954725415906	T	T	T
8.7674535735845005	2.6139213244509762	21.6463547336711812	T	T	T
6.2573925682188651	1.6316726885108339	21.6530296667340458	T	T	T
8.4726352523465991	-0.0442022638193989	21.6447137680858859	T	T	T
5.7011166294168278	0.8484143541608844	21.8052231538307240	T	T	T
8.1927337088623151	3.2634755086558243	22.0798017275417777	T	T	T
8.2239025353688113	0.1699270592970442	22.5581397871280025	T	T	T
5.6469353975758807	2.2868080345964534	8.8276013437729759	F	F	F
8.0891208536402441	2.7314687829575166	8.0391937587954807	F	F	F
8.6179457163001327	0.3372951483296051	8.0000000000000000	F	F	F
2.6220235033829415	4.4325464844928035	12.3918657751636392	F	F	F
5.2200195932898561	5.9336594582123388	16.7027816012770600	T	T	T
2.6181984125360040	4.4291886348141709	18.7909959029545099	T	T	T
5.2207932883280010	5.9315610383350981	10.0985295441362890	F	F	F
2.6219261003263972	7.4333491447405660	14.5561856244294301	F	F	F
2.6583011466075983	4.4477183630247943	9.7781175373791616	F	F	F
5.2194947043667206	5.9348676072154349	14.0665571956713524	F	F	F
2.6267061813961168	7.4312351482512087	18.1807575303043016	T	T	T
2.6230195833822605	4.4361494201313096	16.1094975642247853	T	T	T

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  5.2160668675350168  5.9131246968722753 20.4659241119621029   T   T   T
  2.6280278398637189  7.4322690567836833 11.8834768182986377   F   F   F
  4.2346027215423465  4.4370189614150881 11.0348070799988349   F   F   F
  6.7877002680542313  5.9406754665941532 15.3525199088156761   T   T   T
  4.2002831652051835  7.4526581557904059 19.5619103478012448   T   T   T
  3.4048641426175008  5.7965302555228515 17.4472636957184406   T   T   T
  6.0157760273438523  7.3754382120920763  8.8712015584813955   F   F   F
  3.4199385214817446  8.8113119708011993 13.2250185171475483   F   F   F
  1.8160296701133873  5.8248450066289088 11.0371856277262967   F   F   F
  4.4314511185469483  7.2881334112136216 15.3518763069199267   T   T   T
  1.8194394294860656  8.7975076332755666 19.5622069309588937   T   T   T
  6.2448665053049170  4.4295911424356218 17.4429044055532785   T   T   T
  3.6100736612351203  5.8743990385076188  8.8494658732768272   F   F   F
  1.0323632985175113  7.4351341681358720 13.2250148374957792   F   F   F
  4.4305608419828664  7.5439018708395116 11.0407582029264013   F   F   F
  4.4402576953316775  4.5742834896750617 15.3527726600999941   T   T   T
  1.8359493767284860  6.0392226319948659 19.5630469902082993   T   T   T
  0.8153185185059566  7.5729249735177158 17.4493383247139029   T   T   T
  6.0897215412578829  4.4968913934402082  8.9135372731794220   F   F   F
  3.4185786814707440  6.0526441150753536 13.2221143204608840   F   F   F
  2.6162263120485116  7.4248149947544375 20.7855954725415906   T   T   T
  6.1709815770427880  7.1111427571767400 21.6463547336711812   T   T   T
  3.6609205716771536  6.1288941069508835 21.6530296524483283   T   T   T
  5.8761632700906024  4.4530191403349360 21.6447137680858859   T   T   T
  3.1046446328751163  5.3456357726009340 21.8052231538307240   T   T   T
  5.5962617123206044  7.7606969270958741 22.0798017275417777   T   T   T
  5.6274305388270980  4.6671484777370935 22.5581397871280025   T   T   T
  3.0504634010341687  6.7840294530365028  8.8276013437729759   F   F   F
  5.4926488570985335  7.2286902013975656  8.0391937587954807   F   F   F
  6.0214737197584212  4.8345165667696541  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Ag E_tot= -109.60448298 eV
 D3-zero damping= -12.4169229 eV, D3-BJ damping= -15.7714089 eV
Ag
 1.0000000000000000
    10.3858879861668498    0.0000000000000000    0.0000000000000000
    -5.1929439930834222    8.9944428368800970    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000323980098436  0.0000161467290190  7.8875646103515074
  2.7954954851858491  0.6924502935560881  7.8886013067205907
  8.3884076626024644  2.0747301297338936  7.8885769843793812
  0.7982261246468355  2.7671885389912565  7.8885278624426798
  3.5955832210211884  3.4591520783860181  7.8868784695095666
 -1.1979382834132410  4.8431652720040486  7.8883943167739652
  1.5976283143044490  5.5354403544628665  7.8884392556723766
  4.3949946206649910  6.2272434664654215  7.8886074369616095
 -0.3996679505562832  7.6102898181512826  7.8884756891324184
  2.3975343621723506  8.3022201236126385  7.8885328048476220
  8.7879530794437937  0.4611170599018328 10.2757286857974268
  1.1984990810770146  1.1533803914758975 10.2758796148622960
  6.7910345903884970  2.5371863201873297 10.2740530206427021
 -0.7985438201991050  3.2286294989510007 10.2750428378317906
  1.9983064156203536  3.9222691858811198 10.2741315478896063
  0.0000355203946032  5.9962885281451301 10.2739976319286210
  2.7963532453181434  6.6886192538372979 10.2750326375465484
  0.7970520609008078  8.7638399534066274 10.2740748339834713
 -3.5953713681917954  8.5328266405236270 12.6619918293677944
 -0.3988468181636216  1.6142929138343054 12.6620297287616328
  2.3978114057799544  2.3059039230144740 12.6610992827343871
  7.9891546006726664  3.6911646274855783 12.6605041226791037
  0.4007187800970778  4.3818255575604033 12.6610270019424149
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  3.1948066202481309  5.0731230071890643 12.6605212625088708
 -1.5984196482039481  6.4564853729678742 12.6610335620727952
  1.1979078015087026  7.1504629973387601 12.6610222602256286
  3.9945337900377815  7.8418013397661541 12.6619124713693978
  7.1900598598672012  0.9235821430006279 12.6611798839436176
  5.5924133135037390  1.3843044901982020  7.8868945316795731
  6.3908450560240286  4.1509839940171185  7.8869312230171760
 -3.1955782392037957  6.9196245227568465  7.8884071145575199
 -1.9975067988823123  8.0717883366692948 10.2749943396593899
  3.9947433101423329  1.8445795414764581 10.2740320327309522
  4.7931140788152904  4.6125961219519844 10.2740618468379967
 -2.7952520502311660  5.3026229320910412 10.2741223432374369
  5.5924221223937751  7.3799155629421564 10.2757637578500240
  4.3951690162679364  0.2300774298767013 12.6604592919816632
  5.1930109845758716  2.9980958043038552 12.6614176409864143
  5.9910317637272481  5.7648610201565775 12.6611915316042296

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt13/Cu E_tot= -1173.06459219 eV
 D3-zero damping= -36.5578674 eV, D3-BJ damping= -49.2466349 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Cu
 1.0000000000000000
     9.0995808326891421    0.0000000000000000    0.0000000000000000
    -4.5497904163445693    7.8804681648987556    0.0000000000000000
     0.0000000000000022    0.0000000000000038   35.9489492151250047
  11  18   1   3   3  11  18   1   3   3  11  18   1   3   3  11  18   1
3   3  39
Selective dynamics
Cartesian
  0.0223869159968266 -0.0566648504283547 12.3918657751636410   F   F   F
  2.2974824991582379  1.2594403032431574 16.7524721348810886   T   T   T
  0.0133850306856220 -0.0511488119459606 19.0042821463872507   T   T   T
  2.2992953281763691  1.2566945965667704 10.0985295441362908   F   F   F
  0.0223015764488209  2.5724840876540256 14.5561856244294319   F   F   F
  0.0541715209706047 -0.0433720308572727  9.7781175373791633   F   F   F
  2.2981575757049924  1.2595916421391427 14.0665571956713542   F   F   F
  0.0203770366359371  2.5737905989883090 18.5515925315585477   T   T   T
  0.0229617542097227 -0.0539672466909195 16.3443035231494278   T   T   T
  2.2999979792289569  1.2595515457936539 20.8808808995180719   T   T   T
  0.0276476067751468  2.5715377701428839 11.8834768182986394   F   F   F
  1.4352458804205193 -0.0527462962006500 11.0348070799988349   F   F   F
  3.7040305802364086  1.2535172518842796 15.4332795740122375   T   T   T
  1.4342546316287825  2.5701060974489520 19.9089717844513672   T   T   T
  0.7282129248200367  1.1656276608009319 17.6667813446870383   T   T   T
  2.9958183124317803  2.5217455072424877  8.8712015584813955   F   F   F
  0.7214790123565528  3.7797842373263748 13.2250185171475501   F   F   F
 -0.6837834226640416  1.1631954987575439 11.0371856277262985   F   F   F
  1.5976381869148530  2.4803651752852378 15.4341872711723376   T   T   T
 -0.6716195337677106  3.8356278332739051 19.8940632802682913   T   T   T
  3.1625659994100372 -0.0539007782480317 17.6638028542631886   T   T   T
  0.8880656417930444  1.2066121925700097  8.8494658732768272   F   F   F
 -1.3703915878680988  2.5740480333364228 13.2250148374957810   F   F   F
  1.6069343060173806  2.6693446997414449 11.0407582029264013   F   F   F
  1.5888708403649878  0.0435493793675856 15.4343603865757757   T   T   T
 -0.7028121765186377  1.3560496482630342 19.8896886886380990   T   T   T
 -1.5490781639346862  2.6686823716740342 17.6638450694732647   T   T   T
  3.0606055681745410 -0.0002891509293058  8.9135372731794220   F   F   F
  0.7202875904852494  1.3627813602345642 13.2221143204608858   F   F   F
 -0.0080204560178041  2.5981684902150550 21.1331611099226393   T   T   T
  3.0424475092444085  2.4394288680656326 22.1325992372741958   T   T   T
  0.8768292482751876  1.3704477277824281 22.1320406862772074   T   T   T
  3.0094818832207095 -0.0517410742151234 22.1208528718648978   T   T   T
  0.3977639165786786  2.0035835729568134  8.8276013437729759   F   F   F
  2.5374811940492723  2.3931724485758052  8.0391937587954843   F   F   F
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3.0008103374521946	0.2955206594551278	8.0000000000000000	F	F	F
-2.2525082921754582	3.8835692320210229	12.3918657751636410	F	F	F
0.0203839612514801	5.1991344132523789	16.7542865021170861	T	T	T
-2.2588721560000793	3.8849822751076046	19.0118842760489990	T	T	T
0.0244001200040840	5.1969286790161480	10.0985295441362908	F	F	F
-2.2525936317234643	6.5127181701034038	14.5561856244294319	F	F	F
-2.2207236872016800	3.8968620515921044	9.7781175373791633	F	F	F
0.0232623675327076	5.1998257245885204	14.0665571956713542	F	F	F
-2.2531398777117464	6.5156223301664546	18.5483545501044560	T	T	T
-2.2544456157001065	3.8861276233311930	16.3463316071799341	T	T	T
0.0092109069915445	5.2279626204914287	20.9073131689636220	T	T	T
-2.2472476013971381	6.5117718525922612	11.8834768182986394	F	F	F
-0.8396493277517654	3.8874877862487267	11.0348070799988349	F	F	F
1.4292900186600863	5.1943538770774600	15.4356290810893384	T	T	T
-0.8397979906878222	6.5098392466784842	19.8990377122848869	T	T	T
-1.5507673630428376	5.1063944058740987	17.6686671523609213	T	T	T
0.7209231042594956	6.4619795896918646	8.8712015584813955	F	F	F
-1.5534161958157322	7.7200183197757521	13.2250185171475501	F	F	F
-2.9586786308363267	5.1034295812069210	11.0371856277262985	F	F	F
-0.6765813034668771	6.4205277969535848	15.4355503004100960	T	T	T
-2.9664080634295047	7.7531076070654352	19.9080213411926685	T	T	T
0.8879846670944759	3.8888193380143710	17.6669820536082263	T	T	T
-1.3868295663792405	5.1468462750193869	8.8494658732768272	F	F	F
-3.6452867960403830	6.5142821157858002	13.2250148374957810	F	F	F
-0.6679609021549042	6.6095787821908232	11.0407582029264013	F	F	F
-0.6865873369726230	3.9842248325052299	15.4354656820709231	T	T	T
-2.9897203221343416	5.2902414997957283	19.9065746403036421	T	T	T
-3.8250598978817432	6.6074145178183281	17.6668556179356990	T	T	T
0.7857103600022559	3.9399449315200714	8.9135372731794220	F	F	F
-1.5546076176870356	5.3030154426839404	13.2221143204608858	F	F	F
-2.2893249580431814	6.5137612559936553	21.1323607769341031	T	T	T
0.8559296250569726	6.4023342683960820	22.1420986753027123	T	T	T
-1.4554663238966106	5.2875082576961834	22.1287975412845910	T	T	T
0.6559560313904054	3.9339684423082018	22.2185897325071977	T	T	T
-1.8771312915936065	5.9438176554061899	8.8276013437729759	F	F	F
0.2625859858769876	6.3334065310251830	8.0391937587954843	F	F	F
0.7259151292799098	4.2357547419045050	8.0000000000000000	F	F	F
4.5721773323413979	-0.0566648504283547	12.3918657751636410	F	F	F
6.8469935793783012	1.2594809699678116	16.7544043081542391	T	T	T
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Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Cu E_tot= -1076.28308286
eV
 D3-zero damping= -20.0429941 eV, D3-BJ damping= -29.4318619 eV
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3   6
Selective dynamics
Cartesian
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5.2700780068298201	1.3627813602345642	13.2221143204608840	F	F	F
4.6035851954856275	2.5640548337501037	21.1824270724770081	T	T	T
7.5787759078416350	2.5700989630495688	22.0791158971150949	T	T	T
5.4133129455161502	1.2848474608144447	22.1606718322371705	T	T	T
7.5885019254497887	0.0060262256130262	22.1347027361068385	T	T	T
4.8842866971485135	0.4498722369001176	22.1764354061366831	T	T	T
7.5472271278806655	2.2062327650206228	22.9734336751725614	T	T	T
7.0387883136523026	0.1360485057951922	22.9246615084099687	T	T	T
4.9475543329232501	2.0035835729568134	8.8276013437729759	F	F	F
7.0872716103938433	2.3931724485758052	8.0391937587954807	F	F	F
7.5506007537967657	0.2955206594551278	8.0000000000000000	F	F	F
2.2972821241691128	3.8835692320210229	12.3918657751636392	F	F	F
4.5741752871948194	5.1987380013052835	16.7569238453782390	T	T	T
2.3029692502101549	3.8879706437817987	19.0024406054256936	T	T	T
4.5741905363486559	5.1969286790161480	10.0985295441362890	F	F	F
2.2971967846211072	6.5127181701034029	14.5561856244294301	F	F	F
2.3290667291428910	3.8968620515921053	9.7781175373791616	F	F	F
4.5730527838772783	5.1998257245885204	14.0665571956713524	F	F	F
2.2986085492119859	6.5138922202382679	18.5703346121272403	T	T	T
2.2985280701896129	3.8852474116756621	16.3472873642110272	T	T	T
4.5705795670024001	5.2031474065174121	20.8880861141005134	T	T	T
2.3025428149474334	6.5117718525922612	11.8834768182986377	F	F	F
3.7101410885928057	3.8874877862487280	11.0348070799988349	F	F	F
5.9807192819735615	5.1935414380707687	15.4353562315564261	T	T	T
3.7220271668192595	6.5089888587025122	19.9094075918373150	T	T	T
3.0049826707586362	5.1073544344959361	17.6718344816208877	T	T	T
5.2707135206040672	6.4619795896918655	8.8712015584813955	F	F	F
2.9963742205288391	7.7200183197757521	13.2250185171475483	F	F	F
1.5911117855082448	5.1034295812069219	11.0371856277262967	F	F	F
3.8743063794868506	6.4202164817120604	15.4346266595958230	T	T	T
1.6014912711031886	7.7426837423356414	19.9088082158611641	T	T	T
5.4403991853684364	3.8856259856973905	17.6697619055649184	T	T	T
3.1629608499653310	5.1468462750193877	8.8494658732768272	F	F	F
0.9045036203041876	6.5142821157858002	13.2250148374957792	F	F	F
3.8818295141896670	6.6095787821908232	11.0407582029264013	F	F	F
3.8650867509933380	3.9836925559498257	15.4356429584657704	T	T	T
1.5830167641829038	5.2856199187979156	19.9110043580766529	T	T	T
0.7296684283220021	6.6051130481486755	17.6699986530770872	T	T	T
5.3355007763468274	3.9399449315200719	8.9135372731794220	F	F	F
2.9951827986575359	5.3030154426839422	13.2221143204608840	F	F	F
2.3286899873133424	6.5042889161994815	21.1824270724770081	T	T	T
5.3038806996693504	6.5103330454989461	22.0791158971150949	T	T	T
3.1384177373438655	5.2250815432638227	22.1606718322371705	T	T	T
5.3136067172775041	3.9462603080624041	22.1347027361068385	T	T	T
2.6093914889762289	4.3901063193494956	22.1764354061366831	T	T	T
5.2723319197083800	6.1464668474700002	22.9734336751725614	T	T	T
4.7638931054800171	4.0762825882445703	22.9246615084099687	T	T	T
2.6726591247509650	5.9438176554061908	8.8276013437729759	F	F	F

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  4.8123764022215587  6.3334065310251830  8.0391937587954807   F   F   F
  5.2757055456244810  4.2357547419045058  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Cu E_tot= -145.76161747 eV
 D3-zero damping= -12.2185282 eV, D3-BJ damping= -15.3357517 eV
Cu
 1.0000000000000000
     9.0995808326891421    0.0000000000000000    0.0000000000000000
    -4.5497904163445693    7.8804681648987538    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000156215270264  0.0000282465690322  8.2053024337537526
  2.4493240706182196  0.6056713199316976  8.2049046118465334
  7.3504695036120387  1.8183429543580807  8.2049933642149657
  0.7001176040599204  2.4240493096732174  8.2051052892559611
  3.1508404953214137  3.0314994079203665  8.2036611019753991
 -1.0496386470811279  4.2444281805489981  8.2046426589648629
  1.3988827833441528  4.8491833642054560  8.2046681032109472
  3.8496996851589094  5.4565288388740374  8.2049314165021237
 -0.3491423866165154  6.6673563048046738  8.2046006326582948
  2.1004768915564145  7.2748222582234732  8.2050969138215066
  7.7009135487087503  0.4044359517752665 10.2756754694018593
  1.0497834034087608  1.0090824456405003 10.2756305778561945
  5.9493007475137833  2.2217907314696403 10.2740807374903138
 -0.7007555001912739  2.8298286092537550 10.2747283017980156
  1.7493419904761172  3.4354393403185894 10.2741831117347040
  0.0000745324189116  5.2536481338065766 10.2745747907942526
  2.4495681900757722  5.8586418827739868 10.2747293445966044
  0.6999421766492492  7.6776996896355323 10.2741461193528991
 -3.1503495148943697  7.4758697322515362 12.3458230632283925
 -0.3492584398519966  1.4141718651800339 12.3458211603724894
  2.1003217488172385  2.0214904126046589 12.3440561674857889
  6.9992561514341682  3.2332380063278090 12.3440973530973377
  0.3501032286302939  3.8394527113482706 12.3443851652124028
  2.7999835051290582  4.4447723105843124 12.3440853522806897
 -1.3996774631086242  5.6575529073886859 12.3443792304513806
  1.0497331664169220  6.2638591776251511 12.3443779330138952
  3.4997941572436737  6.8708696878299271 12.3458669849129823
  6.2988189753007440  0.8081029181289996 12.3440940907898504
  4.8988672293895306  1.2129691607406665  8.2036506132511615
  5.5997340275960559  3.6360150088398351  8.2036631599358039
 -2.8005537456569565  6.0621668365315262  8.2050985270287011
 -1.7486107045807255  7.0724555609210755 10.2747000758448088
  3.4993043150038989  1.6172953425276095 10.2740403824412869
  4.2008415060626012  4.0413386344639246 10.2740562360083398
 -2.4492085112619391  4.6476972863990733 10.2741697487456598
  4.8987098112604741  6.4668919095507995 10.2756516120398409
  3.8503997512442183  0.2023840648819068 12.3440702562890259
  4.5498220340550954  2.6268114973318477 12.3453269031943567
  5.2503638023903276  5.0507756607925991 12.3440679013400736

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt13/Pt E_tot= -1276.07586502 eV
 D3-zero damping= -40.6620975 eV, D3-BJ damping= -49.4249979 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Pt
 1.0000000000000000
     9.9890116653035843    0.0000000000000000    0.0000000000000000
    -4.9945058326517904    8.6507378608520078    0.0000000000000000
     0.0000000000000022    0.0000000000000039   36.3575839501467826
  11  18   1   3   3  11  18   1   3   3  11  18   1   3   3  11  18   1
3   3  39
Selective dynamics
Cartesian
```

0.0245751061674327	-0.0622035083097608	12.3918657751636410	F	F	F
2.5161962498163932	1.3752340885334329	16.7208338848221167	T	T	T
0.0199654652350006	-0.0623167360559392	18.8860731061706417	T	T	T
2.5240380054236282	1.3795291470716791	10.0985295441362908	F	F	F
0.0244814251774822	2.8239293691498495	14.5561856244294319	F	F	F
0.0594664704728705	-0.0476113933319686	9.7781175373791633	F	F	F
2.5227890442991794	1.3827093619133761	14.0665571956713542	F	F	F
0.0249424438364770	2.8249922227844295	18.2519901125775057	T	T	T
0.0208154935992614	-0.0623661236925540	16.1796959837497560	T	T	T
2.5107639135123541	1.4223504031188923	20.5928253214254475	T	T	T
0.0303499987167049	2.8228905546339194	11.8834768182986394	F	F	F
1.5755327751578034	-0.0579019383131459	11.0348070799988349	F	F	F
4.0407052167401467	1.3832545048604625	15.3794594848165467	T	T	T
1.5397352367556232	2.7878750550008431	19.6195577926100846	T	T	T
0.7699374860525332	1.2514554420021200	17.5071358872988405	T	T	T
3.2886420396979457	2.7682313891076178	8.8712015584813955	F	F	F
0.7919993682359009	4.1492360508902575	13.2250185171475501	F	F	F
-0.7506192550095521	1.2768910590229883	11.0371856277262985	F	F	F
1.7543857222322821	2.6962101488670944	15.3779777239472022	T	T	T
-0.7546171428170682	4.1172468231956696	19.6018806872891922	T	T	T
3.4893010068036272	-0.0736220665474319	17.5129805375873993	T	T	T
0.9748688668777366	1.3245514808529324	8.8494658732768272	F	F	F
-1.5043393546296964	2.8256461813802818	13.2250148374957810	F	F	F
1.7640027407109125	2.9302575398468891	11.0407582029264013	F	F	F
1.7628330948462771	0.0629449552777353	15.3788358412788533	T	T	T
-0.7678238061122303	1.4542836541295228	19.6847019794368272	T	T	T
-1.7112825778188505	2.9381241750504583	17.4945152914375761	T	T	T
3.3597618709601282	-0.0003174137423445	8.9135372731794220	F	F	F
0.7906914918414196	1.4959852717323936	13.2221143204608858	F	F	F
-0.0436065290040361	2.7925540070039623	20.8469373383789858	T	T	T
3.4032844751205249	2.7595919651626266	21.6571724119770934	T	T	T
0.9394540864434446	1.6242376121832687	21.8771796382900625	T	T	T
3.1335650792785397	0.0652867318653261	21.7659080547472676	T	T	T
0.4366430141999262	2.1994221547853083	8.8276013437729759	F	F	F
2.7855051473130361	2.6270910655609003	8.0391937587954843	F	F	F
3.2941220059820266	0.3244060763800155	8.0000000000000000	F	F	F
-2.4726778101584626	4.2631654221162432	12.3918657751636410	F	F	F
0.0235231450037385	5.7112971037876932	16.7166550764121382	T	T	T
-2.4903829393527444	4.2485376721203156	18.8584067363476322	T	T	T
0.0267850890977330	5.7048980774976830	10.0985295441362908	F	F	F
-2.4727714911484133	7.1492982995758538	14.5561856244294319	F	F	F
-2.4377864458530247	4.2777575370940353	9.7781175373791633	F	F	F
0.0255361279732843	5.7080782923393807	14.0665571956713542	F	F	F
-2.4931047451712733	7.1411084926464712	18.2744105357845612	T	T	T
-2.4717548972480077	4.2626125050157020	16.1690537021870462	T	T	T
0.0071034753720240	5.6789261736513099	20.5020335871418276	T	T	T
-2.4669029176091906	7.1482594850599233	11.8834768182986394	F	F	F
-0.9217201411680918	4.2674669921128574	11.0348070799988349	F	F	F
1.5442632522964270	5.7114290794812304	15.3766753978414670	T	T	T
-0.9113512577889231	7.1622592424689371	19.6745565041001420	T	T	T
-1.7112366997493083	5.5849268567793731	17.5084382975993158	T	T	T
0.7913891233720505	7.0936003195336204	8.8712015584813955	F	F	F
-1.7052535480899944	8.4746049813162596	13.2250185171475501	F	F	F
-3.2478721713354477	5.6022599894489922	11.0371856277262985	F	F	F
-0.7377267068284873	7.0217006622918801	15.3758920912588319	T	T	T
-3.2423639055734004	8.4929615634681710	19.6725825829272125	T	T	T
1.0052555788244826	4.2710241026524463	17.5110319839452728	T	T	T
-1.5223840494481589	5.6499204112789361	8.8494658732768272	F	F	F
-4.0015922709555909	7.1510151118062852	13.2250148374957810	F	F	F
-0.7332501756149828	7.2556264702728939	11.0407582029264013	F	F	F
-0.7320790172025096	4.3888189927387806	15.3765619101240727	T	T	T
-3.2270405644263347	5.8422814514908499	19.6255208929333200	T	T	T
-4.2177593075616349	7.2781957952333673	17.5105229656342658	T	T	T

0.8625089546342327	4.3250515166836596	8.9135372731794220	F	F	F
-1.7065614244844758	5.8213542021583971	13.2221143204608858	F	F	F
-2.4096915569269766	7.1780483858570516	20.8933129534032567	T	T	T
0.9604222736100703	6.7673109211493161	21.9612685840885398	T	T	T
-1.4630275851418142	5.7820776894895243	21.6742563093576415	T	T	T
0.7478340901243302	4.3077617734177185	21.5405627926447565	T	T	T
-2.0606099021259694	6.5247910852113113	8.8276013437729759	F	F	F
0.2882522309871409	6.9524599959869038	8.0391937587954843	F	F	F
0.7968690896561312	4.6497750068060189	8.0000000000000000	F	F	F
5.0190809388192248	-0.0622035083097608	12.3918657751636410	F	F	F
7.5150146115228686	1.3730881654129736	16.7178613503120772	T	T	T
5.0150910813400236	-0.0463705761824175	18.8694440194561821	T	T	T
7.5185438380754208	1.3795291470716791	10.0985295441362908	F	F	F
5.0189872578292745	2.8239293691498495	14.5561856244294319	F	F	F
5.0539723031246622	-0.0476113933319686	9.7781175373791633	F	F	F
7.5172948769509720	1.3827093619133761	14.0665571956713542	F	F	F
5.0139306692773360	2.8187746195175949	18.2526211977463291	T	T	T
5.0176500960529893	-0.0639670624033667	16.1754670436965782	T	T	T
7.4622827427009142	1.3395089439966548	20.6409416310965987	T	T	T
5.0248558313684981	2.8228905546339194	11.8834768182986394	F	F	F
6.5700386078095958	-0.0579019383131459	11.0348070799988349	F	F	F
9.0352670829266959	1.3800258316516920	15.3752727387881389	T	T	T
6.5487566371746597	2.7883889511755653	19.6216968000829652	T	T	T
5.7737180662068175	1.2443133042764052	17.5043924093179903	T	T	T
8.2831478723497387	2.7682313891076178	8.8712015584813955	F	F	F
5.7865052008876940	4.1492360508902575	13.2250185171475501	F	F	F
4.2438865776422396	1.2768910590229883	11.0371856277262985	F	F	F
6.7502914041622875	2.6937021217697645	15.3734572758555128	T	T	T
4.2825405956785447	4.1752604471589247	19.6149278001809186	T	T	T
8.4821880427805159	-0.0663257288590221	17.5194423684499441	T	T	T
5.9693746995295296	1.3245514808529324	8.8494658732768272	F	F	F
3.4901664780220960	2.8256461813802818	13.2250148374957810	F	F	F
6.7585085733627048	2.9302575398468891	11.0407582029264013	F	F	F
6.7577145872562285	0.0604972626984564	15.3768950499459063	T	T	T
4.2267289977919882	1.5121101040557454	19.6133357752779958	T	T	T
3.2780807049141956	2.9541070965737104	17.4982696653314100	T	T	T
8.3542677036119191	-0.0003174137423445	8.9135372731794220	F	F	F
5.7851973244932129	1.4959852717323936	13.2221143204608858	F	F	F
5.0264201391138839	2.8350730459535161	20.8201163230640027	T	T	T
8.3572786006890531	2.5882997828625829	21.7475629796907910	T	T	T
5.8702332208241739	1.4732732251994196	21.7162267702836083	T	T	T
8.0465840265170403	-0.0817625075969751	21.8690033259979124	T	T	T
5.4311488468517179	2.1994221547853083	8.8276013437729759	F	F	F
7.7800109799648283	2.6270910655609003	8.0391937587954843	F	F	F
8.2886278386338201	0.3244060763800155	8.0000000000000000	F	F	F
2.5218280224933300	4.2631654221162432	12.3918657751636410	F	F	F
5.0138549046535932	5.7074720086443129	16.7203449432291222	T	T	T
2.5352186221776547	4.2605593503196655	18.8727648252541336	T	T	T
5.0212909217495261	5.7048980774976830	10.0985295441362908	F	F	F
2.5217343415033793	7.1492982995758538	14.5561856244294319	F	F	F
2.5567193867987679	4.2777575370940353	9.7781175373791633	F	F	F
5.0200419606250772	5.7080782923393807	14.0665571956713542	F	F	F
2.5195640431966941	7.1504989555137106	18.2869551698679800	T	T	T
2.5193550682551291	4.2666421881447780	16.1757480560117202	T	T	T
5.0873289521617631	5.7166673808356281	20.6079148370180647	T	T	T
2.5276029150426020	7.1482594850599233	11.8834768182986394	F	F	F
4.0727856914837011	4.2674669921128574	11.0348070799988349	F	F	F
6.5401686868507785	5.7117178305746084	15.3767195116055930	T	T	T
4.0719165870089684	7.1563967874296752	19.6796762737337474	T	T	T
3.2767234989655489	5.5883424161535853	17.5126605960140829	T	T	T
5.7858949560238422	7.0936003195336204	8.8712015584813955	F	F	F
3.2892522845617980	8.4746049813162596	13.2250185171475501	F	F	F
1.7466336613163451	5.6022599894489922	11.0371856277262985	F	F	F

4.2543498240493971	7.0217217472887015	15.3778020028794362	T	T	T
1.7370742174551552	8.4488285471602698	19.6964459651428001	T	T	T
6.0027181990809027	4.2584195864422441	17.4974537694774881	T	T	T
3.4721217832036335	5.6499204112789361	8.8494658732768272	F	F	F
0.9929135616962008	7.1510151118062852	13.2250148374957810	F	F	F
4.2612556570368101	7.2556264702728939	11.0407582029264013	F	F	F
4.2605977186608737	4.3904531803241555	15.3782396812333459	T	T	T
1.7617141873751205	5.8425907175379486	19.6549978445138116	T	T	T
0.7837808094639298	7.2751441783007333	17.5169787808479853	T	T	T
5.8570147872860252	4.3250515166836596	8.9135372731794220	F	F	F
3.2879444081673168	5.8213542021583971	13.2221143204608858	F	F	F
2.5470268047907387	7.1039054596917692	20.9034833390643620	T	T	T
6.0308707964087622	6.9375781514072177	21.8151645133922010	T	T	T
3.5941915709110672	5.8517034245945805	21.7571904834719305	T	T	T
5.7730057571238556	4.2698257543263232	21.6880971871057184	T	T	T
2.9338959305258236	6.5247910852113113	8.8276013437729759	F	F	F
5.2827580636389335	6.9524599959869038	8.0391937587954843	F	F	F
5.7913749223079236	4.6497750068060189	8.0000000000000000	F	F	F
0.0921139823009864	0.1205331184740040	23.7384584629204660	T	T	T
2.8436036189205707	0.3943939582952880	23.7069098716613560	T	T	T
8.2127143213787406	2.4548772572503843	23.7093242040807759	T	T	T
0.9255085653937684	2.5249263135148396	23.7218486203429606	T	T	T
3.4723119592224165	3.0866720126201286	23.5856568517181771	T	T	T
-1.3455352615978795	5.1435096219193239	23.5597885448370192	T	T	T
1.2986519948958521	5.0345096152046747	23.2663821985901293	T	T	T
3.8085747017038409	5.8712406678411000	23.7260287139111803	T	T	T
-0.0073817198872183	7.4855108772972780	23.7085127916932734	T	T	T
2.5792650433262807	8.3076260201697067	23.7941936245640555	T	T	T
8.7862867941480278	0.8968626181523613	26.0130185196644810	T	T	T
1.5651386417557300	1.3581416279159262	26.0072811334035983	T	T	T
6.8164347638815661	2.8756044071082525	25.9451865153584187	T	T	T
-0.4689837415185160	3.5323681484940663	25.8452341734496009	T	T	T
2.2196107915168852	4.0732419519314043	25.7529631210109891	T	T	T
0.4106045501725011	6.0726832741990826	25.8966815786896483	T	T	T
2.9838745906778770	6.8115654067885743	26.0328555249659885	T	T	T
1.1343407047218321	8.8077228871710425	26.0234265467175767	T	T	T
-2.9527479976386917	8.6922278317697987	28.3212211313709616	T	T	T
0.0911768985246864	2.0678350856431087	28.2215231460360947	T	T	T
2.7757174724054261	2.7369327187611576	28.2203880331802033	T	T	T
8.1553023726711054	4.0612963250277225	28.2249407983632921	T	T	T
0.8545271448738299	4.6958719370810726	28.1702747383104146	T	T	T
3.5221351295643868	5.3824794093732331	28.2905995378746127	T	T	T
-1.0533472219215358	6.6990055763299736	28.3120479141709183	T	T	T
1.6160782556281148	7.3783006714254205	28.3405053632597124	T	T	T
4.3132502429350295	8.0648026571690927	28.3548823268875978	T	T	T
7.3691715494826129	1.4119386548764374	28.2879332232525087	T	T	T
5.6094141300818521	1.4462033640580616	23.6754860991397216	T	T	T
5.9944326449730694	4.1011726665635670	23.6360571677270315	T	T	T
-3.4816095255645299	6.6573101404902477	23.7301541138698404	T	T	T
-1.4783761323185260	8.0284240428258773	25.9960507270416166	T	T	T
4.1847948568980069	2.0931278956980979	25.9476023185117342	T	T	T
4.8445896392249450	4.7887083443810337	25.9635177823530512	T	T	T
-2.4267254565794207	5.5183535978657572	25.9448132157790852	T	T	T
5.6243924551626474	7.4596400934192983	26.0663907106278003	T	T	T
4.6979489218759323	0.7295534781834675	28.3148339821175483	T	T	T
5.4522693358147389	3.4012127703397277	28.2853161406317568	T	T	T
6.2296494805124016	6.0476518047861916	28.3148276648559829	T	T	T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Pt E_tot= -1085.66840113 eV
D3-zero damping= -16.765891 eV, D3-BJ damping= -24.8238239 eV
Al O Al O H Al O Al O H Al O Al O H Al O Al O H
1.0000000000000000

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     9.9890116653035843    0.0000000000000000    0.0000000000000000
    -4.9945058326517904    8.6507378608520078    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.6738067593554113
  11  18   1   3   6  11  18   1   3   6  11  18   1   3   6  11  18   1
3   6
Selective dynamics
Cartesian
  0.0245751061674327 -0.0622035083097608 12.3918657751636392   F   F   F
  2.5217005680874807  1.3805717010303367 16.7203832649988655   T   T   T
  0.0269215653971828 -0.0623976522442425 18.8525726588571807   T   T   T
  2.5240380054236282  1.3795291470716791 10.0985295441362890   F   F   F
  0.0244814251774822  2.8239293691498495 14.5561856244294301   F   F   F
  0.0594664704728705 -0.0476113933319686  9.7781175373791616   F   F   F
  2.5227890442991794  1.3827093619133761 14.0665571956713524   F   F   F
  0.0223410908630030  2.8256249105702902 18.2871470465895705   T   T   T
  0.0240467348954250 -0.0604816501269816 16.1705030995523806   T   T   T
  2.5235170544741132  1.3791644920994286 20.5695969529881388   T   T   T
  0.0303499987167049  2.8228905546339194 11.8834768182986377   F   F   F
  1.5755327751578034 -0.0579019383131459 11.0348070799988349   F   F   F
  4.0429883706401579  1.3850457556096223 15.3747876291625793   T   T   T
  1.5606215046655936  2.8270369670709803 19.6596189434518109   T   T   T
  0.7824224673953224  1.2585057641349238 17.5087350891579057   T   T   T
  3.2886420396979457  2.7682313891076178  8.8712015584813955   F   F   F
  0.7919993682359009  4.1492360508902575 13.2250185171475483   F   F   F
 -0.7506192550095521  1.2768910590229883 11.0371856277262967   F   F   F
  1.7592544917220667  2.6962364492197337 15.3737144689644616   T   T   T
 -0.7363335699810384  4.1435773388978845 19.6491133203633908   T   T   T
  3.5002641912514352 -0.0645128912627999 17.5052756322494893   T   T   T
  0.9748688668777366  1.3245514808529324  8.8494658732768272   F   F   F
 -1.5043393546296964  2.8256461813802818 13.2250148374957792   F   F   F
  1.7640027407109125  2.9302575398468891 11.0407582029264013   F   F   F
  1.7645601378311118  0.0637946461649241 15.3759765477445249   T   T   T
 -0.7440075286793253  1.4875244277123365 19.6561318522962551   T   T   T
 -1.7115232335256036  2.9486835966851617 17.5072313533476915   T   T   T
  3.3597618709601282 -0.0003174137423445  8.9135372731794220   F   F   F
  0.7906914918414196  1.4959852717323936 13.2221143204608840   F   F   F
  0.0543117287842614  2.8084260828221908 20.8999616645970825   T   T   T
  3.3923813905611753  2.6878892493528181 21.7392857722711064   T   T   T
  1.0004510529630488  1.4835001781791988 21.7970534477786941   T   T   T
  3.2154793918379334 -0.0182773978640940 21.7838208978777352   T   T   T
  0.4889187239677378  0.6471983128838446 21.8335458445798736   T   T   T
  3.2809933499737758  2.4643264848488031 22.6737956022125537   T   T   T
  2.7873337085809324  0.1294112802217464 22.6425897484001446   T   T   T
  0.4366430141999262  2.1994221547853083  8.8276013437729759   F   F   F
  2.7855051473130361  2.6270910655609003  8.0391937587954807   F   F   F
  3.2941220059820266  0.3244060763800155  8.0000000000000000   F   F   F
 -2.4726778101584626  4.2631654221162432 12.3918657751636392   F   F   F
  0.0244476517615853  5.7059406314563406 16.7203832649988655   T   T   T
 -2.4703313509287121  4.2629712781817615 18.8525726588571807   T   T   T
  0.0267850890977330  5.7048980774976830 10.0985295441362890   F   F   F
 -2.4727714911484129  7.1492982995758538 14.5561856244294301   F   F   F
 -2.4377864458530247  4.2777575370940353  9.7781175373791616   F   F   F
  0.0255361279732842  5.7080782923393798 14.0665571956713524   F   F   F
 -2.4749118254628923  7.1509938409962945 18.2871470465895705   T   T   T
 -2.4732061814304704  4.2648872802990221 16.1705030995523806   T   T   T
  0.0262641381482180  5.7045334225254321 20.5695969529881388   T   T   T
 -2.4669029176091901  7.1482594850599233 11.8834768182986377   F   F   F
 -0.9217201411680918  4.2674669921128583 11.0348070799988349   F   F   F
  1.5457354543142623  5.7104146717499118 15.3747876291625793   T   T   T
 -0.9366314116603016  7.1524058974969842 19.6596189434518109   T   T   T
 -1.7148304489305728  5.5838746945609277 17.5087350891579057   T   T   T
  0.7913891233720505  7.0936003195336212  8.8712015584813955   F   F   F
 -1.7052535480899942  8.4746049813162614 13.2250185171475483   F   F   F
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-3.2478721713354473	5.6022599894489922	11.0371856277262967	F	F	F
-0.7379984246038284	7.0216053796457381	15.3737144689644616	T	T	T
-3.2335864863069337	8.4689462693238884	19.6491133060776768	T	T	T
1.0030112749255402	4.2608560391632038	17.5052756322494893	T	T	T
-1.5223840494481586	5.6499204112789361	8.8494658732768272	F	F	F
-4.0015922709555918	7.1510151118062861	13.2250148374957792	F	F	F
-0.7332501756149827	7.2556264702728930	11.0407582029264013	F	F	F
-0.7326927784947833	4.3891635765909287	15.3759765477445249	T	T	T
-3.2412604450052207	5.8128933581383402	19.6561318522962551	T	T	T
-4.2087761498514986	7.2740525271111647	17.5072313533476915	T	T	T
0.8625089546342330	4.3250515166836596	8.9135372731794220	F	F	F
-1.7065614244844756	5.8213542021583979	13.2221143204608840	F	F	F
-2.4429411875416336	7.1337950132481946	20.8999616645970825	T	T	T
0.8951284742352803	7.0132581797788216	21.7392857722711064	T	T	T
-1.4968018633628464	5.8088691086052027	21.7970534620644116	T	T	T
0.7182264755120384	4.3070915325619099	21.7838208978777352	T	T	T
-2.0083341923581570	4.9725672433098485	21.8335458445798736	T	T	T
0.7837404336478808	6.7896954152748075	22.6737956022125537	T	T	T
0.2900807922550375	4.4547802106477503	22.6425897484001446	T	T	T
-2.0606099021259690	6.5247910852113122	8.8276013437729759	F	F	F
0.2882522309871409	6.9524599959869047	8.0391937587954807	F	F	F
0.7968690896561315	4.6497750068060197	8.0000000000000000	F	F	F
5.0190809388192248	-0.0622035083097608	12.3918657751636392	F	F	F
7.5162064007392724	1.3805717010303367	16.7203832649988655	T	T	T
5.0214273980489743	-0.0623976522442425	18.8525726588571807	T	T	T
7.5185438380754199	1.3795291470716791	10.0985295441362890	F	F	F
5.0189872578292745	2.8239293691498495	14.5561856244294301	F	F	F
5.0539723031246631	-0.0476113933319686	9.7781175373791616	F	F	F
7.5172948769509720	1.3827093619133761	14.0665571956713524	F	F	F
5.0168469235147954	2.8256249105702902	18.2871470465895705	T	T	T
5.0185525675472169	-0.0604816501269816	16.1705030995523806	T	T	T
7.5180228871259054	1.3791644920994286	20.5695969529881388	T	T	T
5.0248558313684972	2.8228905546339194	11.8834768182986377	F	F	F
6.5700386078095958	-0.0579019383131459	11.0348070799988349	F	F	F
9.0374942032919492	1.3850457556096223	15.3747876291625793	T	T	T
6.5551273373173862	2.8270369670709803	19.6596189434518109	T	T	T
5.7769283000471150	1.2585057641349238	17.5087350891579057	T	T	T
8.2831478723497369	2.7682313891076178	8.8712015584813955	F	F	F
5.7865052008876932	4.1492360508902575	13.2250185171475483	F	F	F
4.2438865776422396	1.2768910590229883	11.0371856277262967	F	F	F
6.7537603243738591	2.6962364492197337	15.3737144689644616	T	T	T
4.2581722626707537	4.1435773388978845	19.6491133060776768	T	T	T
8.4947700239032287	-0.0645128912627999	17.5052756322494893	T	T	T
5.9693746995295287	1.3245514808529324	8.8494658732768272	F	F	F
3.4901664780220960	2.8256461813802818	13.2250148374957792	F	F	F
6.7585085733627048	2.9302575398468891	11.0407582029264013	F	F	F
6.7590659704829035	0.0637946461649241	15.3759765477445249	T	T	T
4.2504983039724671	1.4875244277123365	19.6561318522962551	T	T	T
3.2829825991261883	2.9486835966851617	17.5072313533476915	T	T	T
8.3542677036119208	-0.0003174137423445	8.9135372731794220	F	F	F
5.7851973244932120	1.4959852717323936	13.2221143204608840	F	F	F
5.0488175614360529	2.8084260828221908	20.8999616645970825	T	T	T
8.3868872232129679	2.6878892493528181	21.7392857722711064	T	T	T
5.9949568856148412	1.4835001924649129	21.7970534620644116	T	T	T
8.2099852244897260	-0.0182773978640940	21.7838208978777352	T	T	T
5.4834245566195303	0.6471983128838446	21.8335458445798736	T	T	T
8.2754991826255679	2.4643264848488031	22.6737956022125537	T	T	T
7.7818395412327250	0.1294112802217464	22.6425897484001446	T	T	T
5.4311488468517179	2.1994221547853083	8.8276013437729759	F	F	F
7.7800109799648283	2.6270910655609003	8.0391937587954807	F	F	F
8.2886278386338184	0.3244060763800155	8.0000000000000000	F	F	F
2.5218280224933296	4.2631654221162432	12.3918657751636392	F	F	F
5.0189534844133767	5.7059406314563406	16.7203832649988655	T	T	T

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  2.5241744817230800  4.2629712781817615 18.8525726588571807   T   T   T
  5.0212909217495252  5.7048980774976830 10.0985295441362890   F   F   F
  2.5217343415033793  7.1492982995758538 14.5561856244294301   F   F   F
  2.5567193867987674  4.2777575370940353  9.7781175373791616   F   F   F
  5.0200419606250763  5.7080782923393798 14.0665571956713524   F   F   F
  2.5195940071888998  7.1509938409962945 18.2871470465895705   T   T   T
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  2.5276029150426020  7.1482594850599233 11.8834768182986377   F   F   F
  4.0727856914837002  4.2674669921128583 11.0348070799988349   F   F   F
  6.5402412869660544  5.7104146717499118 15.3747876291625793   T   T   T
  4.0578744209914905  7.1524058974969842 19.6596189434518109   T   T   T
  3.2796753837212194  5.5838746945609277 17.5087350891579057   T   T   T
  5.7858949560238422  7.0936003195336212  8.8712015584813955   F   F   F
  3.2892522845617980  8.4746049813162614 13.2250185171475483   F   F   F
  1.7466336613163449  5.6022599894489922 11.0371856277262967   F   F   F
  4.2565074080479643  7.0216053796457381 15.3737144689644616   T   T   T
  1.7609193463448585  8.4689462693238884 19.6491133203633908   T   T   T
  5.9975171075773321  4.2608560391632038 17.5052756322494893   T   T   T
  3.4721217832036335  5.6499204112789361  8.8494658732768272   F   F   F
  0.9929135616962006  7.1510151118062861 13.2250148374957792   F   F   F
  4.2612556570368092  7.2556264702728930 11.0407582029264013   F   F   F
  4.2618130541570087  4.3891635765909287 15.3759765477445249   T   T   T
  1.7532453876465715  5.8128933581383402 19.6561318522962551   T   T   T
  0.7857296828002934  7.2740525271111647 17.5072313533476915   T   T   T
  5.8570147872860252  4.3250515166836596  8.9135372731794220   F   F   F
  3.2879444081673164  5.8213542021583979 13.2221143204608840   F   F   F
  2.5515646451101586  7.1337950132481946 20.8999616645970825   T   T   T
  5.8896343068870722  7.0132581797788216 21.7392857722711064   T   T   T
  3.4977039692889460  5.8088691086052027 21.7970534477786941   T   T   T
  5.7127323081638313  4.3070915325619099 21.7838208978777352   T   T   T
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  5.7782462662996732  6.7896954152748075 22.6737956022125537   T   T   T
  5.2845866249068294  4.4547802106477503 22.6425897484001446   T   T   T
  2.9338959305258232  6.5247910852113122  8.8276013437729759   F   F   F
  5.2827580636389335  6.9524599959869047  8.0391937587954807   F   F   F
  5.7913749223079236  4.6497750068060197  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Pt E_tot= -240.88255483 eV
 D3-zero damping= -18.780599 eV, D3-BJ damping= -19.9697358 eV
Pt
 1.0000000000000000
     9.9890116653035843    0.0000000000000000    0.0000000000000000
    -4.9945058326517895    8.6507378608520060    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
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  2.6888474287097353  0.6663550351833702  7.9620202979308763
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  5.7627399792126406  5.5457263301146869 12.5909605692330508

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt13/Pd E_tot= -1240.33038891 eV
 D3-zero damping= -36.0761312 eV, D3-BJ damping= -47.002024 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Pd
 1.0000000000000000
     9.9079872356281502    0.0000000000000000    0.0000000000000000
    -4.9539936178140733    8.5805686464259363    0.0000000000000000
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  11  18   1   3   3  11  18   1   3   3  11  18   1   3   3  11  18   1
3   3  39
Selective dynamics
Cartesian
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  0.0332972637627615  2.7928023609294756 18.2926469939093117   T   T   T
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  4.9791035072606071  2.8090322109851034 28.1262214762182694   T   T   T
  5.7517933968722765  5.4350296855386651 28.1158962555610970   T   T   T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Pd E_tot= -1087.75020991
eV
 D3-zero damping= -17.058625 eV, D3-BJ damping= -25.1980163 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H
 1.0000000000000000
     9.9079872356281502    0.0000000000000000    0.0000000000000000
    -4.9539936178140733    8.5805686464259363    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.6985531446493702
  11  18   1   3   6  11  18   1   3   6  11  18   1   3   6  11  18   1
3   6
Selective dynamics
Cartesian
  0.0243757687326446 -0.0616989535095981 12.3918657751636392   F   F   F
  2.5010375100932611  1.3695239360229747 16.7237984060445655   T   T   T
  0.0273397849195409 -0.0614392451359321 18.8651271238619458   T   T   T
  2.5035646346116867  1.3683392950515469 10.0985295441362890   F   F   F
  0.0242828476225538  2.8010234727262997 14.5561856244294301   F   F   F
  0.0589841167609801 -0.0472252003711399  9.7781175373791616   F   F   F
  2.5023258042555447  1.3714937140385159 14.0665571956713524   F   F   F
  0.0219425191425283  2.8026460238212993 18.3111223607269977   T   T   T
  0.0234687374081011 -0.0598329271703912 16.1847405208205650   T   T   T
  2.5028777638700586  1.3694350417299694 20.5948566420956816   T   T   T
  0.0301038190726053  2.7999930844047229 11.8834768182986377   F   F   F
  1.5627530679335617 -0.0574322750785718 11.0348070799988349   F   F   F
  4.0125190893218718  1.3735438372825779 15.3800321942508784   T   T   T
  1.5510940519300676  2.8026724435187282 19.6802586822874694   T   T   T
  0.7773085893279038  1.2499153601703308 17.5229326956157294   T   T   T
  3.2619666933672646  2.7457772788285038  8.8712015584813955   F   F   F
  0.7855751794107426  4.1155801201659115 13.2250185171475483   F   F   F
 -0.7445307150139687  1.2665337410738702 11.0371856277262967   F   F   F
  1.7442333617453194  2.6766171045035407 15.3787106734335399   T   T   T
 -0.7291411520253280  4.1126600507266824 19.6696741436925606   T   T   T
  3.4701120454604415 -0.0638256020539371 17.5193097749163513   T   T   T
```

0.9669613584481019	1.3138075722553846	8.8494658732768272	F	F	F
-1.4921371225840019	2.8027263592815506	13.2250148374957792	F	F	F
1.7496942865013276	2.9064891777783060	11.0407582029264013	F	F	F
1.7487990000555629	0.0615795257708019	15.3812431201988442	T	T	T
-0.7393670943248598	1.4755150515066158	19.6770124259068453	T	T	T
-1.6970480286465004	2.9232860198709050	17.5208876644337828	T	T	T
3.3325096463596333	-0.0003148390864820	8.9135372731794220	F	F	F
0.7842779116672971	1.4838508026271076	13.2221143204608840	F	F	F
0.0541766607172460	2.7866774129135994	20.9231623407591272	T	T	T
3.3577472576987923	2.6835207490130419	21.7678948355835082	T	T	T
0.9865802642039724	1.4630201904664062	21.8270430844538659	T	T	T
3.2034078824721699	-0.0145375353927984	21.8109092471316472	T	T	T
0.4743038116200047	0.6263994896308469	21.8622672546993506	T	T	T
3.2564276187076113	2.4400501016608898	22.6985531446493702	T	T	T
2.7636794356632506	0.1281571177228587	22.6646737383605270	T	T	T
0.4331012472681487	2.1815818587001621	8.8276013437729759	F	F	F
2.7629109234317122	2.6057817946916053	8.0391937587954807	F	F	F
3.2674022096939641	0.3217747032069082	8.0000000000000000	F	F	F
-2.4526210401743920	4.2285853697033700	12.3918657751636392	F	F	F
0.0240407011862245	5.6598082592359429	16.7237984060445655	T	T	T
-2.4496570239874957	4.2288450780770361	18.8651271238619458	T	T	T
0.0265678257046500	5.6586236182645155	10.0985295441362890	F	F	F
-2.4527139612844828	7.0913077959392679	14.5561856244294301	F	F	F
-2.4180126921460565	4.2430591228418280	9.7781175373791616	F	F	F
0.0253289953485081	5.6617780372514837	14.0665571956713524	F	F	F
-2.4550542897645085	7.0929303470342671	18.3111223607269977	T	T	T
-2.4535280714989356	4.2304513960425769	16.1847405208205650	T	T	T
0.0258809549630219	5.6597193649429371	20.5948566420956816	T	T	T
-2.4468929898344314	7.0902774076176911	11.8834768182986377	F	F	F
-0.9142437409734749	4.2328520481343963	11.0348070799988349	F	F	F
1.5355222804148352	5.6638281604955463	15.3800321942508784	T	T	T
-0.9259027569769691	7.0929567667316960	19.6802586822874694	T	T	T
-1.6996882195791327	5.5401996833832987	17.5229326956157294	T	T	T
0.7849698844602280	7.0360616020414719	8.8712015584813955	F	F	F
-1.6914216294962940	8.4058644433788796	13.2250185171475483	F	F	F
-3.2215275239210053	5.5568180642868388	11.0371856277262967	F	F	F
-0.7327634471617173	6.9669014277165093	15.3787106734335399	T	T	T
-3.2061379609323648	8.4029443739396505	19.6696741436925606	T	T	T
0.9931152365534048	4.2264587211590312	17.5193097749163513	T	T	T
-1.5100354504589348	5.6040918954683523	8.8494658732768272	F	F	F
-3.9691339314910383	7.0930106824945192	13.2250148374957792	F	F	F
-0.7273025224057090	7.1967735009912737	11.0407582029264013	F	F	F
-0.7281978088514738	4.3518638489837702	15.3812431201988442	T	T	T
-3.2163639032318967	5.7657993747195837	19.6770124259068453	T	T	T
-4.1740448375535371	7.2135703430838731	17.5208876644337828	T	T	T
0.8555128374525967	4.2899694841264866	8.9135372731794220	F	F	F
-1.6927188972397396	5.7741351258400755	13.2221143204608840	F	F	F
-2.4228201481897909	7.0769617361265675	20.9231623407591272	T	T	T
0.8807504487917557	6.9738050722260105	21.7678948355835082	T	T	T
-1.4904165447030642	5.7533045136793746	21.8270430844538659	T	T	T
0.7264110735651332	4.2757467878201698	21.8109092471316472	T	T	T
-2.0026929972870322	4.9166838128438153	21.8622672546993506	T	T	T
0.7794308098005747	6.7303344248738579	22.6985531446493702	T	T	T
0.2866826267562139	4.4184414409358270	22.6646737383605270	T	T	T
-2.0438955616388879	6.4718661819131302	8.8276013437729759	F	F	F
0.2859141145246755	6.8960661179045735	8.0391937587954807	F	F	F
0.7904054007869274	4.6120590264198764	8.0000000000000000	F	F	F
4.9783693865467198	-0.0616989535095981	12.3918657751636392	F	F	F
7.4550311279073362	1.3695239360229747	16.7237984060445655	T	T	T
4.9813334027336156	-0.0614392451359321	18.8651271238619458	T	T	T
7.4575582524257618	1.3683392950515469	10.0985295441362890	F	F	F
4.9782764654366289	2.8010234727262997	14.5561856244294301	F	F	F
5.0129777345750552	-0.0472252003711399	9.7781175373791616	F	F	F

7.4563194220696198	1.3714937140385159	14.0665571956713524	F	F	F
4.9759361369566033	2.8026460238212993	18.3111223607269977	T	T	T
4.9774623552221762	-0.0598329271703912	16.1847405208205650	T	T	T
7.4568713816841337	1.3694350417299694	20.5948566420956816	T	T	T
4.9840974368866799	2.7999930844047229	11.8834768182986377	F	F	F
6.5167466857476368	-0.0574322750785718	11.0348070799988349	F	F	F
8.9665127071359478	1.3735438372825779	15.3800321942508784	T	T	T
6.5050876697441424	2.8026724435187282	19.6802586822874694	T	T	T
5.7313022071419786	1.2499153601703308	17.5229326956157294	T	T	T
8.2159603111813393	2.7457772788285038	8.8712015584813955	F	F	F
5.7395687972248179	4.1155801201659115	13.2250185171475483	F	F	F
4.2094629028001060	1.2665337410738702	11.0371856277262967	F	F	F
6.6982269795593945	2.6766171045035407	15.3787106734335399	T	T	T
4.2248524657887474	4.1126600507266824	19.6696741436925606	T	T	T
8.4241056632745170	-0.0638256020539371	17.5193097749163513	T	T	T
5.9209549762621769	1.3138075722553846	8.8494658732768272	F	F	F
3.4618564952300730	2.8027263592815506	13.2250148374957792	F	F	F
6.7036879043154025	2.9064891777783060	11.0407582029264013	F	F	F
6.7027926178696378	0.0615795257708019	15.3812431201988442	T	T	T
4.2146265234892155	1.4755150515066158	19.6770124259068453	T	T	T
3.2569455891675747	2.9232860198709050	17.5208876644337828	T	T	T
8.2865032641737084	-0.0003148390864820	8.9135372731794220	F	F	F
5.7382715294813718	1.4838508026271076	13.2221143204608840	F	F	F
5.0081702785313214	2.7866774129135994	20.9231623407591272	T	T	T
8.3117408755128679	2.6835207490130419	21.7678948355835082	T	T	T
5.9405738820180476	1.4630201904664062	21.8270430844538659	T	T	T
8.1574015002862446	-0.0145375353927984	21.8109092471316472	T	T	T
5.4282974294340800	0.6263994896308469	21.8622672546993506	T	T	T
8.2104212365216860	2.4400501016608898	22.6985531446493702	T	T	T
7.7176730534773252	0.1281571177228587	22.6646737383605270	T	T	T
5.3870948650822239	2.1815818587001621	8.8276013437729759	F	F	F
7.7169045412457873	2.6057817946916053	8.0391937587954807	F	F	F
8.2213958275080401	0.3217747032069082	8.0000000000000000	F	F	F
2.5013725776396831	4.2285853697033700	12.3918657751636392	F	F	F
4.9780343190002991	5.6598082592359429	16.7237984060445655	T	T	T
2.5043365938265794	4.2288450780770361	18.8651271238619458	T	T	T
4.9805614435187255	5.6586236182645155	10.0985295441362890	F	F	F
2.5012796565295923	7.0913077959392679	14.5561856244294301	F	F	F
2.5359809256680186	4.2430591228418280	9.7781175373791616	F	F	F
4.9793226131625836	5.6617780372514837	14.0665571956713524	F	F	F
2.4989393280495666	7.0929303470342671	18.3111223607269977	T	T	T
2.5004655463151395	4.2304513960425769	16.1847405208205650	T	T	T
4.9798745727770974	5.6597193649429371	20.5948566420956816	T	T	T
2.5071006279796437	7.0902774076176911	11.8834768182986377	F	F	F
4.0397498768406006	4.2328520481343963	11.0348070799988349	F	F	F
6.4895158982289107	5.6638281604955463	15.3800321942508784	T	T	T
4.0280908608371062	7.0929567667316960	19.6802586822874694	T	T	T
3.2543053982349424	5.5401996833832987	17.5229326956157294	T	T	T
5.7389635022743031	7.0360616020414719	8.8712015584813955	F	F	F
3.2625719883177808	8.4058644433788796	13.2250185171475483	F	F	F
1.7324660938930698	5.5568180642868388	11.0371856277262967	F	F	F
4.2212301706523583	6.9669014277165093	15.3787106734335399	T	T	T
1.7478556568817103	8.4029443739396505	19.6696741436925606	T	T	T
5.9471088543674799	4.2264587211590312	17.5193097749163513	T	T	T
3.4439581673551403	5.6040918954683523	8.8494658732768272	F	F	F
0.9848596863230366	7.0930106824945192	13.2250148374957792	F	F	F
4.2266910954083663	7.1967735009912737	11.0407582029264013	F	F	F
4.2257958089626015	4.3518638489837702	15.3812431201988442	T	T	T
1.7376297145821786	5.7657993747195837	19.6770124259068453	T	T	T
0.7799487802605380	7.2135703430838731	17.5208876644337828	T	T	T
5.8095064552666713	4.2899694841264866	8.9135372731794220	F	F	F
3.2612747205743355	5.7741351258400755	13.2221143204608840	F	F	F
2.5311734696242842	7.0769617361265675	20.9231623407591272	T	T	T

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  5.8347440666058308  6.9738050722260105 21.7678948355835082   T   T   T
  3.4635770731110109  5.7533045136793746 21.8270430844538659   T   T   T
  5.6804046913792083  4.2757467878201698 21.8109092471316472   T   T   T
  2.9513006205270429  4.9166838128438153 21.8622672546993506   T   T   T
  5.7334244276146498  6.7303344248738579 22.6985531446493702   T   T   T
  5.2406762445702890  4.4184414409358270 22.6646737383605270   T   T   T
  2.9100980561751872  6.4718661819131302  8.8276013437729759   F   F   F
  5.2399077323387502  6.8960661179045735  8.0391937587954807   F   F   F
  5.7443990186010030  4.6120590264198764  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Pd E_tot= -203.29086678 eV
 D3-zero damping= -14.1335784 eV, D3-BJ damping= -17.3791559 eV
Pd
 1.0000000000000000
     9.9079872356281502    0.0000000000000000    0.0000000000000000
    -4.9539936178140724    8.5805686464259345    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000804348190537  0.0000299130449570  7.9936653394070518
  2.6668000938447247  0.6604977463985356  7.9942299257631557
  8.0026839546889441  1.9792427764581855  7.9943194798666006
  0.7614427512627229  2.6397108308667354  7.9943438061797245
  3.4296738642570963  3.3003656400083168  7.9936929530415632
 -1.1433433499832180  4.6202337821079045  7.9944228590358515
  1.5244976003531299  5.2802822959778579  7.9944812978140769
  4.1926882507082093  5.9409111877795953  7.9942527662404528
 -0.3810054367097065  7.2607048967346568  7.9943704577043393
  2.2873628551369474  7.9201988218729946  7.9943367342120988
  8.3835364423602279  0.4401737586667512 10.2753727135905280
  1.1435791498117882  1.1001996280509680 10.2753926178517414
  6.4788180259349959  2.4204384901752465 10.2744204594623039
 -0.7614548468274647  3.0805353940403570 10.2749773481867486
  1.9055838157271734  3.7411733384295842 10.2741560087492445
  0.0000608870106830  5.7203816383873232 10.2745057092182623
  2.6669573279511822  6.3808681341793951 10.2749424590986393
  0.7613719864049624  8.3601965415958688 10.2741104984627025
 -3.4295051277264652  8.1399476438472824 12.5556784252318749
 -0.3808394026955591  1.5404883074634019 12.5557160415399824
  2.2871672760056541  2.1996307654225564 12.5546586921569912
  7.6209922453581687  3.5211696283263425 12.5548285934311981
  0.3818766296834039  4.1800119318989459 12.5549654079051756
  3.0481268888229871  4.8392993651978715 12.5548365581039167
 -1.5248075636021066  6.1598706896419069 12.5549411919367664
  1.1431161321909917  6.8211803096437604 12.5549358917431526
  3.8102448470560017  7.4805330704592539 12.5555670991557111
  6.8594469436506680  0.8809469349482081 12.5547603054472638
  5.3350134128532511  1.3199725251857235  7.9936947853810221
  6.0974106551268896  3.9602099041101719  7.9935851064191459
 -3.0486078564774410  6.6013517036288647  7.9942852582296435
 -1.9053351745000715  7.6997329949379480 10.2749011031753792
  3.8108252833779015  1.7595185996001728 10.2743780357200567
  4.5724412025248053  4.4006444975385310 10.2742775480308808
 -2.6667782949926733  5.0596709526469121 10.2741359449358729
  5.3351086132304140  7.0401873165473106 10.2753635192184714
  4.1929685941927293  0.2200380022237894 12.5546762947466579
  4.9540485088940303  2.8601491493486293 12.5562440057503277
  5.7153651913864687  5.4998473058185322 12.5547132063225444

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt13/Ir E_tot= -1382.46849598 eV
 D3-zero damping= -39.393613 eV, D3-BJ damping= -49.274059 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Ir
 1.0000000000000000
```

```
     9.7892996361861151    0.0000000000000000    0.0000000000000000
    -4.8946498180930558    8.4777821701949403    0.0000000000000000
     0.0000000000000022    0.0000000000000038   36.1035259647936826
  11  18   1   3   3  11  18   1   3   3  11  18   1   3   3  11  18   1
3   3  39
Selective dynamics
Cartesian
  0.0240837718409825 -0.0609598628642441 12.3918657751636410   F   F   F
  2.4750536558408478  1.3493391398637442 16.7264408315082242   T   T   T
  0.0297000095861451 -0.0666303965872245 18.9077832698520574   T   T   T
  2.4735744792487950  1.3519479834471189 10.0985295441362908   F   F   F
  0.0239919638311846  2.7674700633352143 14.5561856244294319   F   F   F
  0.0582775470958119 -0.0466594905521906  9.7781175373791633   F   F   F
  2.4723504888190266  1.3550646157062396 14.0665571956713542   F   F   F
  0.0404682006471131  2.7549133343106673 18.3278207858036701   T   T   T
  0.0245888058888762 -0.0595163660953333 16.2100530873059334   T   T   T
  2.4469349523082853  1.4493529204277911 20.6597923194747395   T   T   T
  0.0297432059697828  2.7664520180166585 11.8834768182986394   F   F   F
  1.5440328772689287 -0.0567442948967788 11.0348070799988349   F   F   F
  3.9678631653451339  1.3547157642652392 15.3916152003315752   T   T   T
  1.4893032449223622  2.7927391492353864 19.7277458635823422   T   T   T
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  5.6978348574780640  5.4681014317188303 28.0825184541860580   T   T   T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Ir E_tot= -1089.64695708
eV
 D3-zero damping= -17.4911641 eV, D3-BJ damping= -25.7599733 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H
 1.0000000000000000
     9.7892996361861151    0.0000000000000000    0.0000000000000000
    -4.8946498180930558    8.4777821701949403    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.7365925843185153
  11  18   1   3   6  11  18   1   3   6  11  18   1   3   6  11  18   1
3   6
Selective dynamics
Cartesian
  0.0240837718409825 -0.0609598628642441 12.3918657751636392   F   F   F
  2.4715924551459669  1.3538987937218012 16.7285892501794571   T   T   T
  0.0278194626663782 -0.0593107950178563 18.8852396053544922   T   T   T
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  0.0239919638311846  2.7674700633352143 14.5561856244294301   F   F   F
  0.0582775470958119 -0.0466594905521906  9.7781175373791616   F   F   F
  2.4723504888190266  1.3550646157062396 14.0665571956713524   F   F   F
  0.0225553382714453  2.7695963107230672 18.3471789225312349   T   T   T
  0.0237692407406063 -0.0589836291137393 16.2066865081704172   T   T   T
  2.4722103960321955  1.3544294435369000 20.6326696588039660   T   T   T
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  1.5440328772689287 -0.0567442948967788 11.0348070799988349   F   F   F
  3.9677182429400979  1.3563624251012647 15.3879162895913133   T   T   T
  1.5355374186418056  2.7677300737789312 19.7120710479654377   T   T   T
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  0.7761647885807836  4.0662796605309444 13.2250185171475483   F   F   F
 -0.7356119950787925  1.2513619563545826 11.0371856277262967   F   F   F
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  3.4258060409622186 -0.0618983321060141 17.5402111056451844   T   T   T
  0.9553781458683840  1.2980694951695519  8.8494658732768272   F   F   F
 -1.4742628390482893  2.7691525510432968 13.2250148374957792   F   F   F
  1.7287347303691261  2.8716723966187270 11.0407582029264013   F   F   F
  1.7257055093442357  0.0587303160523976 15.3888722815073837   T   T   T
 -0.7331908520249404  1.4579377404065570 19.7093089158175481   T   T   T
 -1.6746842169390155  2.8863210550161735 17.5415554818157950   T   T   T
  3.2925895737316058 -0.0003110676347737  8.9135372731794220   F   F   F
  0.7748830607841145  1.4660757807679090 13.2221143204608840   F   F   F
  0.0540572816769636  2.7536373570579618 20.9607841960775474   T   T   T
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  3.1844964403378846 -0.0107755463526250 21.8551848926408461   T   T   T
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  3.2282620578692138  0.3179201698716742  8.0000000000000000   F   F   F
 -2.4232411372055456  4.1779312222332257 12.3918657751636392   F   F   F
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 -2.3890473619507162  4.1922315945452793  9.7781175373791616   F   F   F
  0.0250255797724988  5.5939557008037095 14.0665571956713524   F   F   F
 -2.4247695707750827  7.0084873958205378 18.3471789225312349   T   T   T
 -2.4235556683059216  4.1799074559837308 16.2066865081704172   T   T   T
  0.0248854869856676  5.5933205286343703 20.6326696588039660   T   T   T
```

-2.4175817030767450	7.0053431031141287	11.8834768182986377	F	F	F
-0.9032920317775992	4.1821467902006910	11.0348070799988349	F	F	F
1.5203933338935700	5.5952535101987344	15.3879162895913133	T	T	T
-0.9117874904047223	7.0066211588764009	19.7120710479654377	T	T	T
-1.6766913170372471	5.4768215712147255	17.5433998320102482	T	T	T
0.7755667444475063	6.9517767476898555	8.8712015584813955	F	F	F
-1.6711601204657442	8.3051707456284145	13.2250185171475483	F	F	F
-3.1829369041253202	5.4902530414520525	11.0371856277262967	F	F	F
-0.7246925853983621	6.8868667262144267	15.3868730775946965	T	T	T
-3.1672369007622274	8.3067316455515616	19.7031715785189263	T	T	T
0.9784811319156907	4.1769927529914561	17.5402111056451844	T	T	T
-1.4919467631781438	5.5369605802670225	8.8494658732768272	F	F	F
-3.9215877480948169	7.0080436361407674	13.2250148374957792	F	F	F
-0.7185901786774018	7.1105634817161967	11.0407582029264013	F	F	F
-0.7216193997022922	4.2976214011498675	15.3888722815073837	T	T	T
-3.1805157610714683	5.6968288255040269	19.7093089158175481	T	T	T
-4.1220091259855431	7.1252121401136437	17.5415554818157950	T	T	T
0.8452646646850779	4.2385800174626969	8.9135372731794220	F	F	F
-1.6724418482624133	5.7049668658653792	13.2221143204608840	F	F	F
-2.3932676273695641	6.9925284421554323	20.9607841960775474	T	T	T
0.8588609819010768	6.9123123373452664	21.8110426775580102	T	T	T
-1.4812645031685632	5.6701459390272539	21.8715950634959526	T	T	T
0.7371715312913567	4.2281155387448450	21.8551848926408461	T	T	T
-1.9945368804592336	4.8326392395874107	21.9000339466202263	T	T	T
0.7698320359964663	6.6452238166189996	22.7365925843185153	T	T	T
0.2798836563181544	4.3695436469020210	22.7001506354401350	T	T	T
-2.0194117737663282	6.3943398142691299	8.8276013437729759	F	F	F
0.2824891545310351	6.8134582669190067	8.0391937587954807	F	F	F
0.7809371488226859	4.5568112549691442	8.0000000000000000	F	F	F
4.9187335899340399	-0.0609598628642441	12.3918657751636392	F	F	F
7.3662422732390240	1.3538987937218012	16.7285892501794571	T	T	T
4.9224692807594357	-0.0593107950178563	18.8852396053544922	T	T	T
7.3682242973418521	1.3519479834471189	10.0985295441362890	F	F	F
4.9186417819242418	2.7674700633352143	14.5561856244294301	F	F	F
4.9529273651888692	-0.0466594905521906	9.7781175373791616	F	F	F
7.3670003069120842	1.3550646157062396	14.0665571956713524	F	F	F
4.9172051563645027	2.7695963107230672	18.3471789225312349	T	T	T
4.9184190588336643	-0.0589836291137393	16.2066865081704172	T	T	T
7.3668602141252535	1.3544294435369000	20.6326696588039660	T	T	T
4.9243930240628400	2.7664520180166585	11.8834768182986377	F	F	F
6.4386826953619867	-0.0567442948967788	11.0348070799988349	F	F	F
8.8623680610331554	1.3563624251012647	15.3879162895913133	T	T	T
6.4301872367348629	2.7677300737789312	19.7120710479654377	T	T	T
5.6652834101023384	1.2379304861172553	17.5433998320102482	T	T	T
8.1175414715870922	2.7128856625923854	8.8712015584813955	F	F	F
5.6708146066738410	4.0662796605309444	13.2250185171475483	F	F	F
4.1590378230142653	1.2513619563545826	11.0371856277262967	F	F	F
6.6172821417412235	2.6479756411169566	15.3868730775946965	T	T	T
4.1747378263773580	4.0678405604540924	19.7031715785189263	T	T	T
8.3204558590552757	-0.0618983321060141	17.5402111056451844	T	T	T
5.8500279639614412	1.2980694951695519	8.8494658732768272	F	F	F
3.4203869790447685	2.7691525510432968	13.2250148374957792	F	F	F
6.6233845484621838	2.8716723966187270	11.0407582029264013	F	F	F
6.6203553274372933	0.0587303160523976	15.3888722815073837	T	T	T
4.1614589660681176	1.4579377404065570	19.7093089158175481	T	T	T
3.2199656011540423	2.8863210550161735	17.5415554818157950	T	T	T
8.1872393918246633	-0.0003110676347737	8.9135372731794220	F	F	F
5.6695328788771722	1.4660757807679090	13.2221143204608840	F	F	F
4.9487070997700213	2.7536373570579618	20.9607841960775474	T	T	T
8.2008357090406623	2.6734212522477963	21.8110426775580102	T	T	T
5.8607102239710223	1.4312548539297834	21.8715950634959526	T	T	T
8.0791462584309421	-0.0107755463526250	21.8551848926408461	T	T	T
5.3474378466803518	0.5937481544899403	21.9000339466202263	T	T	T

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  8.1118067631360518  2.4063327315215295 22.7365925843185153   T   T   T
  7.6218583834577398  0.1306525618045505 22.7001506354401350   T   T   T
  5.3225629533732572  2.1554487291716597  8.8276013437729759   F   F   F
  7.6244638816706205  2.5745671818215370  8.0391937587954807   F   F   F
  8.1229118759622718  0.3179201698716742  8.0000000000000000   F   F   F
  2.4714086808875120  4.1779312222332257 12.3918657751636392   F   F   F
  4.9189173641924970  5.5927898788192714 16.7285892501794571   T   T   T
  2.4751443717129078  4.1795802900796142 18.8852396053544922   T   T   T
  4.9208993882953251  5.5908390685445895 10.0985295441362890   F   F   F
  2.4713168728777144  7.0063611484326849 14.5561856244294301   F   F   F
  2.5056024561423413  4.1922315945452793  9.7781175373791616   F   F   F
  4.9196753978655563  5.5939557008037095 14.0665571956713524   F   F   F
  2.4698802473179748  7.0084873958205378 18.3471789225312349   T   T   T
  2.4710941497871359  4.1799074559837308 16.2066865081704172   T   T   T
  4.9195353050787247  5.5933205286343703 20.6326696588039660   T   T   T
  2.4770681150163125  7.0053431031141287 11.8834768182986377   F   F   F
  3.9913577863154583  4.1821467902006910 11.0348070799988349   F   F   F
  6.4150431519866276  5.5952535101987344 15.3879162895913133   T   T   T
  3.9828623276883350  7.0066211588764009 19.7120710479654377   T   T   T
  3.2179585010558105  5.4768215712147255 17.5433998320102482   T   T   T
  5.6702165625405634  6.9517767476898555  8.8712015584813955   F   F   F
  3.2234896976273131  8.3051707456284145 13.2250185171475483   F   F   F
  1.7117129139677372  5.4902530414520525 11.0371856277262967   F   F   F
  4.1699572326946956  6.8868667262144267 15.3868730775946965   T   T   T
  1.7274129173308299  8.3067316455515616 19.7031715785189263   T   T   T
  5.8731309500087487  4.1769927529914561 17.5402111056451844   T   T   T
  3.4027030549149138  5.5369605802670225  8.8494658732768272   F   F   F
  0.9730620699982404  7.0080436361407674 13.2250148374957792   F   F   F
  4.1760596394156559  7.1105634817161967 11.0407582029264013   F   F   F
  4.1730304183907654  4.2976214011498675 15.3888722815073837   T   T   T
  1.7141340570215893  5.6968288255040269 19.7093089158175481   T   T   T
  0.7726406921075142  7.1252121401136437 17.5415554818157950   T   T   T
  5.7399144827781354  4.2385800174626969  8.9135372731794220   F   F   F
  3.2222079698306443  5.7049668658653792 13.2221143204608840   F   F   F
  2.5013821907234934  6.9925284421554323 20.9607841960775474   T   T   T
  5.7535107999941344  6.9123123373452664 21.8110426775580102   T   T   T
  3.4133853149244944  5.6701459390272539 21.8715950634959526   T   T   T
  5.6318213493844143  4.2281155387448450 21.8551848926408461   T   T   T
  2.9001129376338239  4.8326392395874107 21.9000339466202263   T   T   T
  5.6644818540895239  6.6452238166189996 22.7365925843185153   T   T   T
  5.1745334744112119  4.3695436469020210 22.7001506354401350   T   T   T
  2.8752380443267294  6.3943398142691299  8.8276013437729759   F   F   F
  5.1771389726240926  6.8134582669190067  8.0391937587954807   F   F   F
  5.6755869669157430  4.5568112549691442  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Ir E_tot= -338.60687474 eV
 D3-zero damping= -17.3430281 eV, D3-BJ damping= -18.8938231 eV
Ir
 1.0000000000000000
     9.7892996361861151    0.0000000000000000    0.0000000000000000
    -4.8946498180930549    8.4777821701949385    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000339838607237  0.0000149689493741  8.1022092024089538
  2.6354221359004910  0.6522360181626565  8.1012089165750449
  7.9067901601629069  1.9562165936200098  8.1012418181822792
  0.7529855489465405  2.6085435658787981  8.1013251254128651
  3.3886170685453898  3.2606294367178346  8.1007597948498198
 -1.1293978350082048  4.5648055375861674  8.1013777841543479
  1.5061491412019270  5.2173121997853817  8.1013979028178689
  4.1418212141843798  5.8693755731893873  8.1012353840134121
 -0.3766666991144472  7.1735053313813770  8.1013689757231298
```

```
  2.2591662025786539  7.8256402630238524  8.1013215467351944
  8.2832841574688612  0.4352443942661725 10.2751948556196577
  1.1300527952782971  1.0866588531537928 10.2751621351987161
  6.4007639914355732  2.3911004439254016 10.2743682422214011
 -0.7530095655332623  3.0435982281693645 10.2744233115862045
  1.8825703157316118  3.6953834289035594 10.2746941107823115
  0.0000401411746834  5.6518516112484134 10.2745237901068602
  2.6353922177309168  6.3038301063250017 10.2744336408766728
  0.7531236719969402  8.2604041827730370 10.2746829026872177
 -3.3885974866468809  8.0422751971075268 12.4482991716437734
 -0.3757694716661100  1.5219705122372462 12.4482958971987454
  2.2596706474058936  2.1735532731296590 12.4481390381976880
  7.5305559405516798  3.4781726711039975 12.4478073995758756
  0.3769846091451847  4.1302885136182095 12.4478682636697151
  3.0119113794394718  4.7824898793033883 12.4478131369400220
 -1.5060920836187310  6.0861729046250836 12.4478750938555454
  1.1293052745269108  6.7390077533098971 12.4478603527519311
  3.7645672717533039  7.3912918629067166 12.4483106195874722
  6.7771903158020130  0.8700514738007019 12.4481745287637136
  5.2712528847385531  1.3043153931106848  8.1007521853615909
  6.0241356747397816  3.9128533610989185  8.1007756569137630
 -3.0120500298796626  6.5214322682412105  8.1013079220898891
 -1.8822443272911806  7.6081252946450979 10.2744132659560261
  3.7651002692881335  1.7389940810990501 10.2743334628870908
  4.5181892219417596  4.3476251827669934 10.2743650313614285
 -2.6355792765824653  4.9997372597502272 10.2746973856614900
  5.2707419809848108  6.9558553464760751 10.2751686235465076
  4.1416660126175184  0.2170460005446599 12.4477935700548290
  4.8947039763361309  2.8258896062873697 12.4480040985242102
  5.6472782643916135  5.4341081583626867 12.4481521140061169

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt13/Rh E_tot= -1321.69079544 eV
 D3-zero damping= -36.7160517 eV, D3-BJ damping= -47.7989383 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Rh
 1.0000000000000000
     9.6544501462291485    0.0000000000000000    0.0000000000000000
    -4.8272250731145725    8.3609990862048331    0.0000000000000000
     0.0000000000000022    0.0000000000000038   36.0226256574897263
  11  18   1   3   3  11  18   1   3   3  11  18   1   3   3  11  18   1
3   3  39
Selective dynamics
Cartesian
  0.0237520132402966 -0.0601201289996575 12.3918657751636392   F   F   F
  2.4383069450525521  1.3307789359541868 16.7333910022908690   T   T   T
  0.0198722049744857 -0.0587645836246861 18.9193006688424425   T   T   T
  2.4395005138688548  1.3333246393069225 10.0985295441362890   F   F   F
  0.0236614699035351  2.7293476296186667 14.5561856244294301   F   F   F
  0.0574747626481111 -0.0460167470734481  9.7781175373791616   F   F   F
  2.4382933841432530  1.3363983393557579 14.0665571956713524   F   F   F
  0.0308619957210254  2.7205650814386271 18.3722247304632766   T   T   T
  0.0232264500782265 -0.0577036718338781 16.2326503286327508   T   T   T
  2.3978470717853888  1.4245761839017430 20.7037712499592637   T   T   T
  0.0293334875727809  2.7283436080706629 11.8834768182986377   F   F   F
  1.5227635266805732 -0.0559626312937450 11.0348070799988331   F   F   F
  3.9154659425845457  1.3347014599760505 15.4008623727092342   T   T   T
  1.4617920771598492  2.7553861348443824 19.7460039354077459   T   T   T
  0.7618396099771795  1.2203210877785187 17.5624549333223534   T   T   T
  3.1784956995635079  2.6755151395204533  8.8712015584813937   F   F   F
  0.7654729689662547  4.0102658741903907 13.2250185171475483   F   F   F
 -0.7254787980137113  1.2341242041315126 11.0371856277262967   F   F   F
  1.6941783659127876  2.6158269516043196 15.3972392776175582   T   T   T
 -0.7541169135307808  4.0457070965185462 19.8072650375805424   T   T   T
  3.3726940785228381 -0.0742824453026275 17.5712447610444755   T   T   T
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0.9422176277032074	1.2801883375936554	8.8494658732768254	F	F	F
-1.4539545841887389	2.7310069407341713	13.2250148374957792	F	F	F
1.7049210761420710	2.8321145556700151	11.0407582029263995	F	F	F
1.6994367571276090	0.0546464108123243	15.3993101794794747	T	T	T
-0.7593178687145586	1.4237546740066391	19.7273293466419268	T	T	T
-1.6411158536672656	2.8518572440038059	17.5697929341194978	T	T	T
3.2472335175113964	-0.0003067826181279	8.9135372731794202	F	F	F
0.7642088972171138	1.4458803042147124	13.2221143204608840	F	F	F
-0.0958175228879362	2.6968262981226063	20.9747139577311650	T	T	T
3.2410292350236900	2.7644025415637490	21.7927008677313729	T	T	T
0.8687554617185735	1.5017613533310132	21.9215639928028629	T	T	T
3.0530836918900173	0.1406642897154463	21.8685311051824840	T	T	T
0.4220185493360615	2.1257570073366514	8.8276013437729741	F	F	F
2.6922103485181061	2.5391020224913197	8.0391937587954825	F	F	F
3.1837921255829551	0.3135407582337105	7.9999999999999982	F	F	F
-2.3898605233169898	4.1203794141027590	12.3918657751636392	F	F	F
0.0219002371886280	5.5157263956144238	16.7353320444305744	T	T	T
-2.3985383938528306	4.1097996215020531	18.9270118463930004	T	T	T
0.0258879773115682	5.5138241824093388	10.0985295441362890	F	F	F
-2.3899510666537513	6.9098471727210828	14.5561856244294301	F	F	F
-2.3561377739091753	4.1344827960289683	9.7781175373791616	F	F	F
0.0246808475859667	5.5168978824581751	14.0665571956713524	F	F	F
-2.4046465529727326	6.9045040154435551	18.3733163025834685	T	T	T
-2.3889991045169037	4.1278235206057836	16.2368480043044379	T	T	T
0.0189567332587176	5.5124187098842752	20.7229014525604676	T	T	T
-2.3842790489845056	6.9088431511730786	11.8834768182986377	F	F	F
-0.8908490098767131	4.1245369118086703	11.0348070799988331	F	F	F
1.5013867973338317	5.5167445378974564	15.3996575222102461	T	T	T
-0.8645174993874468	6.9192246397954484	19.8126096412881196	T	T	T
-1.6442867164523787	5.4059354092611214	17.5797920601476676	T	T	T
0.7648831630062216	6.8560146826228685	8.8712015584813937	F	F	F
-1.6481395675910318	8.1907654172928073	13.2250185171475483	F	F	F
-3.1390913345709976	5.4146237472339287	11.0371856277262967	F	F	F
-0.7157627776547097	6.7956838320872324	15.3991696254141015	T	T	T
-3.1339074442377908	8.2342179301720133	19.7285068572588962	T	T	T
0.9502577511532772	4.1279226178093076	17.5792415181241140	T	T	T
-1.4713949088540792	5.4606878806960708	8.8494658732768254	F	F	F
-3.8675671207460249	6.9115064838365869	13.2250148374957792	F	F	F
-0.7086914604152154	7.0126140987724321	11.0407582029263995	F	F	F
-0.7151752051170742	4.2366281023296457	15.3999187796317312	T	T	T
-3.0892303677991468	5.6453560717476030	19.7488380168182829	T	T	T
-4.0683453955947426	7.0223719410906549	17.5627394150995997	T	T	T
0.8336209809541096	4.1801927604842879	8.9135372731794202	F	F	F
-1.6494036393401728	5.6263798473171276	13.2221143204608840	F	F	F
-2.3644755370194432	7.0230670006225111	20.9766200615002063	T	T	T
1.0274934251348251	6.5668373344290254	22.1079537350083406	T	T	T
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Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Rh E_tot= -1090.47435722
eV
 D3-zero damping= -17.9891104 eV, D3-BJ damping= -26.4222289 eV
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3   6
Selective dynamics
Cartesian
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6.5248289391630578	2.6153201990741963	15.3961603032204142	T	T	T
4.1169360264317874	4.0168748640792247	19.7414688323736804	T	T	T
8.2017738280826489	-0.0602308241037325	17.5648837872102241	T	T	T
5.7694427008177813	1.2801883375936554	8.8494658732768272	F	F	F
3.3732704889258356	2.7310069407341713	13.2250148374957792	F	F	F
6.5321461492566453	2.8321145556700151	11.0407582029264013	F	F	F
6.5259553333237434	0.0552040581002685	15.3982679506423441	T	T	T
4.1004510305256279	1.4373178337345212	19.7462807691064306	T	T	T
3.1768335937805849	2.8432765054903588	17.5661094971796423	T	T	T
8.0744585906259712	-0.0003067826181279	8.9135372731794220	F	F	F
5.5914339703316882	1.4458803042147124	13.2221143204608840	F	F	F
4.8803720554037984	2.7168671884772255	21.0030503272270934	T	T	T
8.0753126740321246	2.6602360034110206	21.8598780260504917	T	T	T
5.7701317674601338	1.3982742093600735	21.9239164003067764	T	T	T
7.9877102350676275	-0.0066406054299094	21.9061829824383842	T	T	T
5.2555802106067437	0.5599704284638262	21.9480717464045512	T	T	T
7.9979054833705474	2.3724306430110733	22.7800669120826598	T	T	T
7.5121853678783044	0.1317024868187833	22.7415723283191582	T	T	T
5.2492436224506358	2.1257570073366514	8.8276013437729759	F	F	F
7.5194354216326804	2.5391020224913197	8.0391937587954807	F	F	F
8.0110171986975303	0.3135407582337105	8.0000000000000000	F	F	F
2.4373645497975844	4.1203794141027590	12.3918657751636392	F	F	F
4.8505797441353291	5.5154479304640986	16.7344708073130342	T	T	T
2.4410699092013499	4.1228140789290597	18.9084835050076130	T	T	T
4.8531130504261428	5.5138241824093388	10.0985295441362890	F	F	F
2.4372740064608229	6.9098471727210828	14.5561856244294301	F	F	F
2.4710872992053989	4.1344827960289683	9.7781175373791616	F	F	F
4.8519059207005411	5.5168978824581743	14.0665571956713524	F	F	F
2.4358028827768941	6.9115344423642755	18.3883647704534603	T	T	T
2.4363609407719644	4.1224452981490565	16.2331680068095068	T	T	T
4.8502096779175572	5.5172954743995852	20.6784656119007551	T	T	T
2.4429460241300691	6.9088431511730795	11.8834768182986377	F	F	F
3.9363760632378613	4.1245369118086712	11.0348070799988349	F	F	F
6.3300553296355933	5.5171789583286088	15.3973115947793051	T	T	T
3.9311433849642881	6.9083475662932292	19.7483402905037799	T	T	T
3.1753104720883409	5.4041216240925074	17.5685304736603634	T	T	T
5.5921082361207954	6.8560146826228703	8.8712015584813955	F	F	F
3.1790855055235427	8.1907654172928073	13.2250185171475483	F	F	F
1.6881337385435766	5.4146237472339287	11.0371856277262967	F	F	F
4.1112164026057716	6.7958197421766133	15.3961603032204142	T	T	T
1.7033234898745013	8.1973744071816412	19.7414688323736804	T	T	T
5.7881612915253626	4.1202687189986840	17.5648837872102241	T	T	T
3.3558301642604955	5.4606878806960717	8.8494658732768272	F	F	F
0.9596579523685491	6.9115064838365878	13.2250148374957792	F	F	F

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  4.1185336126993590  7.0126140987724312 11.0407582029264013   F   F   F
  4.1123427967664572  4.2357036012026850 15.3982679506423441   T   T   T
  1.6868384939683412  5.6178173768369373 19.7462807691064306   T   T   T
  0.7632210572232989  7.0237760485927758 17.5661094971796423   T   T   T
  5.6608460540686849  4.1801927604842888  8.9135372731794220   F   F   F
  3.1778214337744020  5.6263798473171285 13.2221143204608840   F   F   F
  2.4667595188465121  6.8973667315796421 21.0030503272270934   T   T   T
  5.6617001374748384  6.8407355465134376 21.8598780260504917   T   T   T
  3.3565192309028475  5.5787737524624905 21.9239164003067764   T   T   T
  5.5740976985103412  4.1738589376725068 21.9061829824383842   T   T   T
  2.8419676740494575  4.7404699715662426 21.9480717464045512   T   T   T
  5.5842929468132612  6.5529301861134899 22.7800669120826598   T   T   T
  5.0985728313210181  4.3122020299211998 22.7415723283191582   T   T   T
  2.8356310858933496  6.3062565504390680  8.8276013437729759   F   F   F
  5.1058228850753942  6.7196015655937362  8.0391937587954807   F   F   F
  5.5974046621402431  4.4940403013361268  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Rh E_tot= -277.28069999 eV
 D3-zero damping= -14.0778022 eV, D3-BJ damping= -16.9893653 eV
Rh
 1.0000000000000000
     9.6544501462291485    0.0000000000000000    0.0000000000000000
    -4.8272250731145716    8.3609990862048331    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000595648638128 -0.0000085203602106  8.1230690787395101
  2.5998163836544905  0.6455386810131792  8.1287576323857706
  7.7955095430323054  1.9286988041673827  8.1287392128467655
  0.7405145685190203  2.5735756149399247  8.1285748837571195
  3.3415484227378824  3.2155913323643102  8.1291824235854939
 -1.1140254899281161  4.5019013223224000  8.1280897812842809
  1.4855724006486479  5.1451698620332182  8.1281399197442923
  4.0864906795501863  5.7868029449552409  8.1288083134268696
 -0.3713634255742174  7.0747957555630103  8.1281180786926193
  2.2282499240553886  7.7154348156918413  8.1284876832066804
  8.1709119259437291  0.4294531318497110 10.2735233912507216
  1.1138757216666775  1.0701008504778671 10.2735315212716234
  6.3108709375801837  2.3575100658463830 10.2757993369002971
 -0.7447230087870993  3.0025300096002385 10.2746158781096337
  1.8546910249098179  3.6433991225840110 10.2747762659344328
  0.0000045729888670  5.5739818226771725 10.2740833696928888
  2.5994441761340434  6.2149583195965041 10.2747510914237896
  0.7445772328021770  8.1455342145698033 10.2746051699363825
 -3.3414595495415580  7.9325917347971941 12.4203356308503086
 -0.3717990720693223  1.5008020276200185 12.4203067105500331
  2.2274251586084919  2.1415938537880486 12.4206670701707047
  7.4263656801983613  3.4324114326535562 12.4206793596118708
  0.3715232362571894  4.0735301490339522 12.4209961814629661
  2.9688913989359289  4.7150478358545316 12.4207024776054986
 -1.4853569867798770  6.0026513886511967 12.4208756731908121
  1.1137498373307297  6.6461036709587606 12.4209630410783003
  3.7134475550966561  7.2886206563388818 12.4202532221798183
  6.6861700889445252  0.8580621426428959 12.4206294822331493
  5.1989187027395287  1.2859190519408177  8.1291817630956889
  5.9412556514895405  3.8593803239334554  8.1291634922416840
 -2.9686756174601605  6.4329216120338453  8.1286117568021901
 -1.8545850998154769  7.5047023123500827 10.2746273944173563
  3.7135541740037299  1.7169328786401377 10.2758447556461530
  4.4574249902453067  4.2865053699543330 10.2758309839117992
 -2.5992009342452773  4.9330403250247992 10.2746067046675886
  5.1969182372625147  6.8613896043097515 10.2735048923818457
  4.0866531965823611  0.2134413703448029 12.4207834110590145
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  4.8273764954661296  2.7869455810838399 12.4262439433424454
  5.5683431582806442  5.3611697492689316 12.4206755223701730

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt13/Os E_tot= -1466.95248272 eV
 D3-zero damping= -35.3449066 eV, D3-BJ damping= -46.708316 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Os
 1.0000000000000000
     9.7653265728439838    0.0000000000000000    0.0000000000000000
    -4.8826632864219901    8.4570208883341209    0.0000000000000000
     0.0000000000000022    0.0000000000000038   36.0857865064111323
  11  18   1   3   3  11  18   1   3   3  11  18   1   3   3  11  18   1
3   3  39
Selective dynamics
Cartesian
  0.0240247929753518 -0.0608105779605141 12.3918657751636410   F   F   F
  2.4662986619606819  1.3494933830427760 16.7266718914553003   T   T   T
  0.0256547876629867 -0.0535519115210246 18.8919316672247106   T   T   T
  2.4675169307135238  1.3486371914755828 10.0985295441362908   F   F   F
  0.0239332097946342  2.7606927924791309 14.5561856244294319   F   F   F
  0.0581348309281723 -0.0465452258995504  9.7781175373791633   F   F   F
  2.4662959377198534  1.3517461913988533 14.0665571956713542   F   F   F
  0.0240657048838088  2.7523101700035286 18.3360222705405782   T   T   T
  0.0245577507602804 -0.0571401271806373 16.2076287366451517   T   T   T
  2.4533965338075729  1.4516950198208780 20.6285681668700747   T   T   T
  0.0296703676884746  2.7596772402566918 11.8834768182986394   F   F   F
  1.5402516876695957 -0.0566053335178833 11.0348070799988349   F   F   F
  3.9585057031438398  1.3529859847689136 15.3942084459305732   T   T   T
  1.4754350844732373  2.7687214084029712 19.7151226768918519   T   T   T
  0.7669826515279654  1.2338073317898390 17.5389603336262603   T   T   T
  3.2149990984977155  2.7062420637399316  8.8712015584813955   F   F   F
  0.7742640348668205  4.0563217285550559 13.2250185171475501   F   F   F
 -0.7338105512974551  1.2482974899924812 11.0371856277262985   F   F   F
  1.7148626958403477  2.6444398622554335 15.3900544382577600   T   T   T
 -0.7660113401682578  4.0886630897368956 19.7470974468612965   T   T   T
  3.4181418281204450 -0.0682813752324010 17.5476011001442807   T   T   T
  0.9530385156948495  1.2948906464891867  8.8494658732768272   F   F   F
 -1.4706525096338323  2.7623711599349079 13.2250148374957810   F   F   F
  1.7245012235062154  2.8646399441634443 11.0407582029264013   F   F   F
  1.7215981278653736  0.0586830590880494 15.3907307295168501   T   T   T
 -0.7666407188192172  1.4448669780915844 19.6918342510337112   T   T   T
 -1.6639644603580761  2.8893118160781412 17.5433962101955530   T   T   T
  3.2845263351604896 -0.0003103058597347  8.9135372731794220   F   F   F
  0.7729854458995670  1.4624855006801696 13.2221143204608858   F   F   F
 -0.1174610808408383  2.7585072480178594 20.9386888908821405   T   T   T
  3.2754654396221290  2.7920371859087205 21.7567267926325449   T   T   T
  0.7963635056936808  1.5035124300409586 21.9244895503798780   T   T   T
  3.0297893752512590  0.1822736572090506 21.8274506948681974   T   T   T
  0.4268652167284903  2.1501702403281739  8.8276013437729759   F   F   F
  2.7231290086818607  2.5682623117672758  8.0391937587954843   F   F   F
  3.2203563512635829  0.3171416136262507  8.0000000000000000   F   F   F
 -2.4173068502356436  4.1676998662065463 12.3918657751636410   F   F   F
  0.0222455700617118  5.5832915590110170 16.7330351988515815   T   T   T
 -2.4274455793924252  4.1689950415869621 18.9035076377919538   T   T   T
  0.0261852875025285  5.5771476356426426 10.0985295441362908   F   F   F
 -2.4173984334163610  6.9892032366461914 14.5561856244294319   F   F   F
 -2.3831968122828227  4.1819652182675089  9.7781175373791633   F   F   F
  0.0249642945088581  5.5802566355659140 14.0665571956713542   F   F   F
 -2.4272776840471275  6.9993863328643222 18.3426524095692400   T   T   T
 -2.4158604319721002  4.1754524370062231 16.2140348825259473   T   T   T
  0.0334856171905227  5.5729422012850103 20.6584915857235423   T   T   T
 -2.4116612755225209  6.9881876844237514 11.8834768182986394   F   F   F
 -0.9010799555413995  4.1719051106491758 11.0348070799988349   F   F   F
  1.5156226707603098  5.5822774767367127 15.3935516760249520   T   T   T
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-0.8652807143890511	7.0122585938362718	19.7659554134526907	T	T	T
-1.6684732746996536	5.4745513819964735	17.5641026297954532	T	T	T
0.7736674552867205	6.9347525079069907	8.8712015584813955	F	F	F
-1.6670676083441747	8.2848321727221155	13.2250185171475501	F	F	F
-3.1751421945084504	5.4768079341595417	11.0371856277262985	F	F	F
-0.7224788062421563	6.8715588586327572	15.3939750025743294	T	T	T
-3.1628580113880616	8.3302238946772782	19.6936341827529766	T	T	T
0.9652482287086862	4.1747151240773306	17.5609369254426575	T	T	T
-1.4882931275161457	5.5234010906562467	8.8494658732768272	F	F	F
-3.9119841528448274	6.9908816041019675	13.2250148374957810	F	F	F
-0.7168304197047798	7.0931503883305052	11.0407582029264013	F	F	F
-0.7207968069199461	4.2892495193556632	15.3942365636366603	T	T	T
-3.1187593379903866	5.7264051031433745	19.7487959683161414	T	T	T
-4.1112794860905142	7.1079043849416141	17.5437195236050947	T	T	T
0.8431946919494941	4.2282001383073249	8.9135372731794220	F	F	F
-1.6683461973114284	5.6909959448472289	13.2221143204608858	F	F	F
-2.3463152634635489	7.1174660305323512	20.9540261368196141	T	T	T
1.0581872618186707	6.6251261537276269	22.0553162635591846	T	T	T
-1.3519226984543300	5.9217160864957989	22.0140440029812403	T	T	T
0.5840084687559924	4.2065928415564278	21.8651749139030898	T	T	T
-2.0144664264825054	6.3786806844952331	8.8276013437729759	F	F	F
0.2817973654708651	6.7967727559343354	8.0391937587954843	F	F	F
0.7790247080525874	4.5456520577933102	8.0000000000000000	F	F	F
4.9066880793973437	-0.0608105779605141	12.3918657751636410	F	F	F
7.3498106094830939	1.3556274229709824	16.7264972798839544	T	T	T
4.9098786702551021	-0.0437501094450412	18.9063858176637289	T	T	T
7.3501802171355166	1.3486371914755828	10.0985295441362908	F	F	F
4.9065964962166264	2.7606927924791309	14.5561856244294319	F	F	F
4.9407981173501643	-0.0465452258995504	9.7781175373791633	F	F	F
7.3489592241418462	1.3517461913988533	14.0665571956713542	F	F	F
4.9059723305702008	2.7648335740805763	18.3273186356195907	T	T	T
4.9095405703302646	-0.0601062356689736	16.2151245276597074	T	T	T
7.2675797350446780	1.3093217690596684	20.6383828223251307	T	T	T
4.9123336541104674	2.7596772402566918	11.8834768182986394	F	F	F
6.4229149740915874	-0.0566053335178833	11.0348070799988349	F	F	F
8.8399412577164540	1.3536263677143854	15.3904011190031191	T	T	T
6.3999780757171481	2.7187808439645211	19.6530022348424360	T	T	T
5.6553076100924438	1.2221589363440173	17.5430605708267500	T	T	T
8.0976623849197082	2.7062420637399316	8.8712015584813955	F	F	F
5.6569273212888129	4.0563217285550559	13.2250185171475501	F	F	F
4.1488527351245370	1.2482974899924812	11.0371856277262985	F	F	F
6.5998829460775568	2.6440097583415807	15.3936584085928025	T	T	T
4.1961188738117494	4.0845137113446190	19.6536380010980416	T	T	T
8.2947726632095584	-0.0587862138947378	17.5441542872512315	T	T	T
5.8357018021168425	1.2948906464891867	8.8494658732768272	F	F	F
3.4120107767881596	2.7623711599349079	13.2250148374957810	F	F	F
6.6071645099282073	2.8646399441634443	11.0407582029264013	F	F	F
6.6038130822090837	0.0562219785395529	15.3908279880571364	T	T	T
4.1166443242164146	1.4898631369048507	19.6526649604483943	T	T	T
3.2004439465987060	2.8862031107872537	17.5373387908672882	T	T	T
8.1671896215824802	-0.0003103058597347	8.9135372731794220	F	F	F
5.6556487323215601	1.4624855006801696	13.2221143204608858	F	F	F
4.8993392798993067	2.7613354664939553	20.9072557418883349	T	T	T
8.0784522667152920	2.4615930117729943	21.8229081040649788	T	T	T
5.6852260915787971	1.3436774274487360	21.7606108919217931	T	T	T
8.0430635131269010	-0.1384039982084197	21.9227483365267659	T	T	T
5.3095285031504824	2.1501702403281739	8.8276013437729759	F	F	F
7.6057922951038526	2.5682623117672758	8.0391937587954843	F	F	F
8.1030196376855752	0.3171416136262507	8.0000000000000000	F	F	F
2.4653564361863491	4.1676998662065463	12.3918657751636410	F	F	F
4.9032460070483994	5.5836320830522963	16.7260549042554345	T	T	T
2.4726434607826566	4.1672408010207702	18.9032601044724373	T	T	T
4.9088485739245211	5.5771476356426426	10.0985295441362908	F	F	F

2.4652648530056309	6.9892032366461914	14.5561856244294319	F	F	F
2.4994664741391692	4.1819652182675089	9.7781175373791633	F	F	F
4.9076275809308507	5.5802566355659140	14.0665571956713542	F	F	F
2.4722921897374159	6.9944046193121778	18.3373349377052861	T	T	T
2.4616802917015175	4.1711939027137950	16.2134452428722220	T	T	T
4.9984384056774465	5.5386214168470183	20.6372284682053078	T	T	T
2.4710020108994719	6.9881876844237514	11.8834768182986394	F	F	F
3.9815833308805932	4.1719051106491758	11.0348070799988349	F	F	F
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Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Os E_tot= -1089.9120977 eV
 D3-zero damping= -17.5789952 eV, D3-BJ damping= -25.8754515 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H
 1.0000000000000000
     9.7653265728439838    0.0000000000000000    0.0000000000000000
    -4.8826632864219901    8.4570208883341209    0.0000000000000000
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  11  18   1   3   6  11  18   1   3   6  11  18   1   3   6  11  18   1
3   6
Selective dynamics
Cartesian
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  5.6213272177252405  4.2190228067796562 21.8643401827097001   T   T   T
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  5.6496629126735112  6.6295037880413537 22.7445165036361203   T   T   T
  5.1607303819945640  4.3601158815279408 22.7075587727339290   T   T   T
  2.8681968599394869  6.3786806844952348  8.8276013437729759   F   F   F
  5.1644606518928580  6.7967727559343363  8.0391937587954807   F   F   F
  5.6616879944745797  4.5456520577933111  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Os E_tot= -420.81793684 eV
 D3-zero damping= -13.927276 eV, D3-BJ damping= -16.4082713 eV
Os
 1.0000000000000000
     9.7653265728439838    0.0000000000000000    0.0000000000000000
    -4.8826632864219892    8.4570208883341191    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000580564602431  0.0000147117525127  8.1288116317869203
  2.6291109972467988  0.6511467105944518  8.1279691743055302
  7.8869236020559050  1.9512838947946729  8.1280204094859467
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  0.7509139434441066  2.6024895021468915  8.1281048803221569
  3.3799875435301261  3.2526774765617423  8.1272474493063882
 -1.1268826598130040  4.5531386767420727  8.1280258250481499
  1.5030123721035495  5.2045912150296232  8.1280365222545008
  4.1320724800509128  5.8546273451230872  8.1280062246426397
 -0.3760369461908245  7.1563849670378694  8.1279941307844474
  2.2534594880658774  7.8060998178673904  8.1280987694864990
  8.2628800578295412  0.4335885595407760 10.2755173941801772
  1.1267965444002168  1.0843993930996607 10.2754102028646166
  6.3851967430090912  2.3856641413108646 10.2740080460216152
 -0.7509290784148651  3.0356859252750512 10.2746970547003862
  1.8783219543904282  3.6862081102077289 10.2746090567766473
  0.0000461613893696  5.6379993649153830 10.2742491945469006
  2.6292046739487289  6.2888193781543649 10.2746920449253416
  0.7512162092344642  8.2405421547974171 10.2745583194364798
 -3.3802556265444594  8.0226081824489039 12.4219504862423591
 -0.3749005283809244  1.5182776440462826 12.4219571036873990
  2.2544020402196647  2.1678717429065757 12.4213831492936162
  7.5122338632377481  3.4699137195857346 12.4211570652394201
  0.3760852873754901  4.1196902338042767 12.4210966177821263
  3.0042397668201155  4.7707707653702256 12.4211599393648768
 -1.5028543092660809  6.0714887253039578 12.4210903719783765
  1.1269339703543975  6.7227938652427319 12.4210846841952041
  3.7553607609439261  7.3731473021511515 12.4219801241280337
  6.7608117628949191  0.8683317992179636 12.4214131472757057
  5.2584802307299956  1.3008239358246030  8.1272402973884219
  6.0095742489885637  3.9035180926969577  8.1272503584515459
 -3.0042658433341596  6.5054814002766221  8.1280794074242966
 -1.8781496050171897  7.5895095346276236 10.2746643660085901
  3.7561838873394455  1.7344444220281932 10.2739893248828214
  4.5067035722909621  4.3368329349098849 10.2740044104415436
 -2.6294170905261662  4.9872468047325276 10.2746023829010635
  5.2584589601385296  6.9389940248238533 10.2754355124971397
  4.1316590227394903  0.2162771084611642 12.4211078007147080
  4.8827224691832365  2.8189699949915767 12.4210285413543406
  5.6329521806657539  5.4207891977545835 12.4214050407794989

Interface: O-a-Al2O3(0001)/fcc(111)_sqrt13/Ru E_tot= -1395.03605799 eV
 D3-zero damping= -36.1370926 eV, D3-BJ damping= -47.2488713 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Ru
 1.0000000000000000
     9.6131018524371505    0.0000000000000000    0.0000000000000000
    -4.8065509262185735    8.3251904133778218    0.0000000000000000
     0.0000000000000022    0.0000000000000038   36.0175638143215622
  11  18   1   3   3  11  18   1   3   3  11  18   1   3   3  11  18   1
3   3  39
Selective dynamics
Cartesian
  0.0236502875897690 -0.0598626451741637 12.3918657751636427   F   F   F
  2.4296911835927801  1.3314883476622212 16.7339793219677411   T   T   T
  0.0274334978553096 -0.0566600917010076 18.9258840767403171   T   T   T
  2.4290525668159013  1.3276142468898358 10.0985295441362926   F   F   F
  0.0235601320340238  2.7176583188924583 14.5561856244294336   F   F   F
  0.0572286084564580 -0.0458196655257135  9.7781175373791651   F   F   F
  2.4278506070123340  1.3306747828277459 14.0665571956713560   F   F   F
  0.0245025296947849  2.7156987126554810 18.3775708014788819   T   T   T
  0.0262028118666480 -0.0567999966879861 16.2407853667487103   T   T   T
  2.4445329252974086  1.4181028297399019 20.7078458959752787   T   T   T
  0.0292078574598555  2.7166585973902686 11.8834768182986412   F   F   F
  1.5162418011837029 -0.0557229532918848 11.0348070799988367   F   F   F
  3.9010328819925060  1.3319675465373444 15.4028401251357305   T   T   T
  1.4697800686727054  2.7421475723132662 19.7729543278572635   T   T   T
  0.7602763895529622  1.2216449161263361 17.5689891889331236   T   T   T
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3.1648827674947162	2.6640563837800202	8.8712015584813972	F	F	F
0.7621945843113801	3.9930906183199357	13.2250185171475518	F	F	F
-0.7223717012836243	1.2288386695443176	11.0371856277263003	F	F	F
1.6884518801626163	2.6072061563465256	15.4003653561155982	T	T	T
-0.7383558398657525	4.0371702734261383	19.7855529697171200	T	T	T
3.3620828745562763	-0.0610283950719492	17.5715291336770996	T	T	T
0.9381822770932621	1.2747055185112466	8.8494658732768290	F	F	F
-1.4477275551610174	2.7193105234734158	13.2250148374957828	F	F	F
1.6976192022413574	2.8199851124674757	11.0407582029264031	F	F	F
1.6923179634216070	0.0548130700815903	15.4017677117356619	T	T	T
-0.7458516686547787	1.4254627249862639	19.7368550376932284	T	T	T
-1.6354936676329546	2.8407926310960767	17.5696325161777516	T	T	T
3.2333261935872337	-0.0003054687227085	8.9135372731794238	F	F	F
0.7609359263568382	1.4396878558928281	13.2221143204608875	F	F	F
-0.0673320745659130	2.7058321359914066	20.9687086485635099	T	T	T
3.2494630052704254	2.7333188923639664	21.8250109028741797	T	T	T
0.8719648997149659	1.4810620541894468	21.9580934819056743	T	T	T
3.0732846896204133	0.1302062097532083	21.8638677504970076	T	T	T
0.4202111189076765	2.1166527679508298	8.8276013437729777	F	F	F
2.6806800901652923	2.5282274998821963	8.0391937587954860	F	F	F
3.1701565098630198	0.3121979189015009	8.0000000000000018	F	F	F
-2.3796251755195179	4.1027325615147472	12.3918657751636427	F	F	F
0.0221483159944850	5.4958260122871634	16.7363648500694673	T	T	T
-2.3893370356284067	4.1153424491739079	18.9328211331317533	T	T	T
0.0257771037066144	5.4902094535787462	10.0985295441362926	F	F	F
-2.3797153310752632	6.8802535255813693	14.5561856244294336	F	F	F
-2.3460468546528288	4.1167755411631974	9.7781175373791651	F	F	F
0.0245751439030471	5.4932699895166577	14.0665571956713560	F	F	F
-2.3841163640919656	6.8911797635502703	18.3866177464049727	T	T	T
-2.3789770762208255	4.1083278202574292	16.2440996797085333	T	T	T
0.0072935102016014	5.5154443380912825	20.6967710086775867	T	T	T
-2.3740676056494316	6.8792538040791795	11.8834768182986412	F	F	F
-0.8870336619255841	4.1068722533970252	11.0348070799988367	F	F	F
1.4968521378439110	5.4945789070066047	15.4038813692406027	T	T	T
-0.8669709182502906	6.8989830945537705	19.7847719887438132	T	T	T
-1.6404765473571257	5.3902091056434536	17.5853169512062628	T	T	T
0.7616073043854293	6.8266515904689307	8.8712015584813972	F	F	F
-1.6410808787979068	8.1556858250088453	13.2250185171475518	F	F	F
-3.1256471643929111	5.3914338762332283	11.0371856277263003	F	F	F
-0.7116329580642140	6.7691005518760674	15.4030838211337979	T	T	T
-3.1143757045642526	8.2132924947335741	19.7382477831054715	T	T	T
0.9505379037995926	4.1113287304056936	17.5831425663979140	T	T	T
-1.4650931860160248	5.4373007252001573	8.8494658732768290	F	F	F
-3.8510030182703039	6.8819057301623259	13.2250148374957828	F	F	F
-0.7056562608679295	6.9825803191563871	11.0407582029264031	F	F	F
-0.7119592682173337	4.2193193936147839	15.4031390540473314	T	T	T
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-4.0479870319498241	6.9960680696151867	17.5746820826727408	T	T	T
0.8300507304779469	4.1622897379662023	8.9135372731794238	F	F	F
-1.6423395367524487	5.6022830625817388	13.2221143204608875	F	F	F
-2.3493664071082181	6.9963047092911443	20.9823194346288346	T	T	T
0.9730024329042399	6.5902942642208719	22.0149744400025078	T	T	T
-1.4317085361295221	5.7945502480338718	22.0692160926218328	T	T	T
0.4791335880180443	4.1402742437137992	22.0407130399886064	T	T	T
-1.9830643442016107	6.2792479746397394	8.8276013437729777	F	F	F
0.2774046270560051	6.6908227065711072	8.0391937587954860	F	F	F
0.7668810467537329	4.4747931255904119	8.0000000000000018	F	F	F
4.8302012138083441	-0.0598626451741637	12.3918657751636427	F	F	F
7.2376949267772090	1.3331320017989823	16.7352094606069315	T	T	T
4.8366967915863341	-0.0354563384417152	18.9312288312863046	T	T	T
7.2356034930344775	1.3276142468898358	10.0985295441362926	F	F	F
4.8301110582525997	2.7176583188924583	14.5561856244294336	F	F	F
4.8637795346750332	-0.0458196655257135	9.7781175373791651	F	F	F

7.2344015332309102	1.3306747828277459	14.0665571956713560	F	F	F
4.8336653567294841	2.7222626760528148	18.3832353568771971	T	T	T
4.8324954484690723	-0.0567920545469190	16.2437157849986349	T	T	T
7.1936258101018105	1.3120745720441762	20.7149147999490211	T	T	T
4.8357587836784317	2.7166585973902686	11.8834768182986412	F	F	F
6.3227927274022777	-0.0557229532918848	11.0348070799988367	F	F	F
8.7071978920391899	1.3301382073423271	15.4031606073307472	T	T	T
6.3200596006724776	2.6910365486560077	19.7048056401930545	T	T	T
5.5722730483949023	1.2112080780404868	17.5680436585429902	T	T	T
7.9714336937132924	2.6640563837800202	8.8712015584813972	F	F	F
5.5687455105299559	3.9930906183199357	13.2250185171475518	F	F	F
4.0841792249349513	1.2288386695443176	11.0371856277263003	F	F	F
6.4973388025354524	2.6063626271316069	15.4020820410357633	T	T	T
4.1226586355513053	4.0332127921449654	19.7128114444825648	T	T	T
8.1663402763406285	-0.0613190633300809	17.5805257162137565	T	T	T
5.7447332033118386	1.2747055185112466	8.8494658732768290	F	F	F
3.3588233710575581	2.7193105234734158	13.2250148374957828	F	F	F
6.5041701284599327	2.8199851124674757	11.0407582029264031	F	F	F
6.4998416573735378	0.0523671024292936	15.4029800027284178	T	T	T
4.0690579176170392	1.4688977405045682	19.6994825971660461	T	T	T
3.1560401675089502	2.8398221097439547	17.5679711780331047	T	T	T
8.0398771198058085	-0.0003054687227085	8.9135372731794238	F	F	F
5.5674868525754144	1.4396878558928281	13.2221143204608875	F	F	F
4.8539207322531199	2.7274806355635994	20.9725054643691493	T	T	T
8.0005266869286285	2.4945248769285735	21.8883027681275095	T	T	T
5.6655671172022597	1.3375976772009350	21.8228521430326410	T	T	T
7.9782092728777920	-0.1023347070634829	21.9737709998569457	T	T	T
5.2267620451262520	2.1166527679508298	8.8276013437729777	F	F	F
7.4872310163838671	2.5282274998821963	8.0391937587954860	F	F	F
7.9767074360815959	0.3121979189015009	8.0000000000000018	F	F	F
2.4269257506990578	4.1027325615147472	12.3918657751636427	F	F	F
4.8287585338001335	5.4954878617845058	16.7333092961005399	T	T	T
2.4364641915461251	4.1064466627566976	18.9304156153566687	T	T	T
4.8323280299251907	5.4902094535787462	10.0985295441362926	F	F	F
2.4268355951433120	6.8802535255813693	14.5561856244294336	F	F	F
2.4605040715657469	4.1167755411631974	9.7781175373791651	F	F	F
4.8311260701216225	5.4932699895166577	14.0665571956713560	F	F	F
2.4265183107083002	6.8802880410067875	18.3829163275604657	T	T	T
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2.4324833205691445	6.8792538040791795	11.8834768182986412	F	F	F
3.9195172642929919	4.1068722533970252	11.0348070799988367	F	F	F
6.3054126612353265	5.4962239432385802	15.4015262620617559	T	T	T
3.9497461255917004	6.8492746911392359	19.7735524665518412	T	T	T
3.1567532205445437	5.3877308014344027	17.5744302155115015	T	T	T
5.5681582306040038	6.8266515904689307	8.8712015584813972	F	F	F
3.1654700474206687	8.1556858250088453	13.2250185171475518	F	F	F
1.6809037618256646	5.3914338762332283	11.0371856277263003	F	F	F
4.0937298168616358	6.7694269628095585	15.4020275571984548	T	T	T
1.7078874781907760	8.1340170268047025	19.7778354211669622	T	T	T
5.7689313822154356	4.1160460372320751	17.5684418613684628	T	T	T
3.3414577402025505	5.4373007252001573	8.8494658732768290	F	F	F
0.9555479079482713	6.8819057301623259	13.2250148374957828	F	F	F
4.1008946653506468	6.9825803191563871	11.0407582029264031	F	F	F
4.0942355914354209	4.2187963746060682	15.4029336150876635	T	T	T
1.6814379385131339	5.5768893678208649	19.7870349206156355	T	T	T
0.7603922321501329	6.9916882525702393	17.5869225361486663	T	T	T
5.6366016566965227	4.1622897379662023	8.9135372731794238	F	F	F
3.1642113894661268	5.6022830625817388	13.2221143204608875	F	F	F
2.4938149230659659	6.8413829195262608	20.9757682522858104	T	T	T
5.7096833423006901	6.8168742522248360	21.9773887711343079	T	T	T
3.3604270324754442	5.5281206713741193	21.9628563404546426	T	T	T
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  2.8234865820169657  6.2792479746397394  8.8276013437729777   F   F   F
  5.0839555532745804  6.6908227065711072  8.0391937587954860   F   F   F
  5.5734319729723092  4.4747931255904119  8.0000000000000018   F   F   F
  0.1196529831113918  0.0078592833040815 23.2314255055932612   T   T   T
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  3.4559439790654602  3.1309704720923621 23.7418655689050127   T   T   T
 -0.9526279416989055  4.5167466467385839 23.6229488478824905   T   T   T
  1.7511611477497340  5.1295919392322205 23.3581497939654064   T   T   T
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  8.3018143435681573  0.4614691891094175 25.9069935055653637   T   T   T
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  6.4510261368714081  2.3609670192371741 25.8740867877006764   T   T   T
 -0.5578679373975737  3.0100280610128896 25.8614558211315746   T   T   T
  2.0169489870425323  3.6485149707549760 25.8159895892533946   T   T   T
  0.1643955441784940  5.5479554861915883 25.8067555376863673   T   T   T
  2.7590108868735204  6.1925203777546942 25.8638349681709414   T   T   T
  0.8808892444182733  8.1012834505523124 25.8736147062096471   T   T   T
 -3.1722360288876215  7.9238569042891722 28.0160436274105464   T   T   T
 -0.2064237615271692  1.4959457141664987 28.0126215133362741   T   T   T
  2.3571617916082328  2.1549592665580493 27.9322116728115120   T   T   T
  7.5679641678908007  3.4332944625128401 28.0041095443968509   T   T   T
  0.5441101286670360  4.0830433563772743 27.9690592859372558   T   T   T
  3.1242506823992273  4.7025352997429817 27.9948988658945161   T   T   T
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  3.8656697084324536  7.2505101306735709 27.9977694910091728   T   T   T
  6.8456165496091419  0.8503158532768464 27.9994522372534043   T   T   T
  5.4056852391071519  1.2794752597798564 23.7553935840254695   T   T   T
  6.0222866657118130  3.8698842662097825 23.7479858485582156   T   T   T
 -2.8570476690659676  6.3650948592242873 23.7744394652173661   T   T   T
 -1.6750227454512863  7.4617680704932159 25.8264868037859792   T   T   T
  3.8865615499049300  1.7073860950183644 25.8492789274303760   T   T   T
  4.5898456758473483  4.2610882168991377 25.8610066100510849   T   T   T
 -2.4111077917892012  4.8981010890317300 25.8354634719944869   T   T   T
  5.3560571626462501  6.8299059815999810 25.8848859098370099   T   T   T
  4.2356569618306059  0.2266073483602499 28.0078332459332842   T   T   T
  4.9696961944135030  2.7786802758197120 28.0097290330211379   T   T   T
  5.7334777170451776  5.3632592840959115 27.9697408309165958   T   T   T

Oxide reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Ru E_tot= -1090.44697535
eV
 D3-zero damping= -18.14119 eV, D3-BJ damping= -26.6286797 eV
Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H Al  O Al  O  H
 1.0000000000000000
     9.6131018524371505    0.0000000000000000    0.0000000000000000
    -4.8065509262185735    8.3251904133778218    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.7943947977984465
  11  18   1   3   6  11  18   1   3   6  11  18   1   3   6  11  18   1
3   6
Selective dynamics
Cartesian
  0.0236502875897690 -0.0598626451741637 12.3918657751636392   F   F   F
  2.4275663757031696  1.3287808198334001 16.7363282806881735   T   T   T
  0.0281241169814450 -0.0580745367475879 18.9161918041684380   T   T   T
  2.4290525668159013  1.3276142468898358 10.0985295441362890   F   F   F
  0.0235601320340238  2.7176583188924583 14.5561856244294301   F   F   F
  0.0572286084564580 -0.0458196655257135  9.7781175373791616   F   F   F
  2.4278506070123340  1.3306747828277459 14.0665571956713524   F   F   F
  0.0231988318167853  2.7184704073296491 18.4018781467768058   T   T   T
```

0.0231956375243801	-0.0581836675391766	16.2413945506665875	T	T	T
2.4266535405976892	1.3302519705926044	20.6938462991109269	T	T	T
0.0292078574598555	2.7166585973902686	11.8834768182986377	F	F	F
1.5162418011837029	-0.0557229532918848	11.0348070799988349	F	F	F
3.9008403781538874	1.3302664638227784	15.4001274447179952	T	T	T
1.5124484054132803	2.7149240662459526	19.7605263347910878	T	T	T
0.7599161601873550	1.2184880831617189	17.5763743565881363	T	T	T
3.1648827674947162	2.6640563837800202	8.8712015584813955	F	F	F
0.7621945843113801	3.9930906183199357	13.2250185171475483	F	F	F
-0.7223717012836243	1.2288386695443176	11.0371856277262967	F	F	F
1.6904565285306394	2.6049174903475518	15.3991011228151855	T	T	T
-0.7067492844507998	3.9998606995920762	19.7541047828348120	T	T	T
3.3596483444785576	-0.0603679293857846	17.5729566469362233	T	T	T
0.9381822770932621	1.2747055185112466	8.8494658732768272	F	F	F
-1.4477275551610174	2.7193105234734158	13.2250148374957792	F	F	F
1.6976192022413574	2.8199851124674757	11.0407582029264013	F	F	F
1.6908566934970581	0.0541354568959082	15.4009141179224649	T	T	T
-0.7234669522761129	1.4297606086376711	19.7589204208876623	T	T	T
-1.6421873167399357	2.8295179560596382	17.5743152541748024	T	T	T
3.2333261935872337	-0.0003054687227085	8.9135372731794220	F	F	F
0.7609359263568382	1.4396878558928281	13.2221143204608840	F	F	F
0.0538114777222623	2.7043881868460646	21.0169952551160435	T	T	T
3.2315157278577469	2.6541788020418196	21.8758425090511430	T	T	T
0.9370011010431682	1.3874361459802860	21.9417599199225393	T	T	T
3.1534933066552333	-0.0063873153032344	21.9231162338119070	T	T	T
0.4216512342858652	0.5490660538412827	21.9641347631205122	T	T	T
3.1562566847262361	2.3607362154158902	22.7943947977984465	T	T	T
2.6715540345689948	0.1319595234285929	22.7549879813096787	T	T	T
0.4202111189076765	2.1166527679508298	8.8276013437729759	F	F	F
2.6806800901652923	2.5282274998821963	8.0391937587954807	F	F	F
3.1701565098630198	0.3121979189015009	8.0000000000000000	F	F	F
-2.3796251755195179	4.1027325615147472	12.3918657751636392	F	F	F
0.0242909125938828	5.4913760265223113	16.7363282806881735	T	T	T
-2.3751513461278417	4.1045206699413228	18.9161918041684380	T	T	T
0.0257771037066146	5.4902094535787462	10.0985295441362890	F	F	F
-2.3797153310752628	6.8802535255813693	14.5561856244294301	F	F	F
-2.3460468546528288	4.1167755411631974	9.7781175373791616	F	F	F
0.0245751439030473	5.4932699895166568	14.0665571956713524	F	F	F
-2.3800766312925012	6.8810656140185600	18.4018781467768058	T	T	T
-2.3800798255849065	4.1044115391497344	16.2413945506665875	T	T	T
0.0233780774884025	5.4928471772815151	20.6938462991109269	T	T	T
-2.3740676056494312	6.8792538040791795	11.8834768182986377	F	F	F
-0.8870336619255839	4.1068722533970261	11.0348070799988349	F	F	F
1.4975649150446007	5.4928616705116893	15.4001274447179952	T	T	T
-0.8908270576960065	6.8775192729348635	19.7605263347910878	T	T	T
-1.6433593029219318	5.3810832898506300	17.5763743565881363	T	T	T
0.7616073043854295	6.8266515904689307	8.8712015584813955	F	F	F
-1.6410808787979065	8.1556858250088471	13.2250185171475483	F	F	F
-3.1256471643929111	5.3914338762332283	11.0371856277262967	F	F	F
-0.7128189345786473	6.7675126970364623	15.3991011228151855	T	T	T
-3.1100247475600864	8.1624559062809876	19.7541047828348120	T	T	T
0.9563728813692709	4.1022272773031263	17.5729566469362233	T	T	T
-1.4650931860160248	5.4373007252001573	8.8494658732768272	F	F	F
-3.8510030182703039	6.8819057301623268	13.2250148374957792	F	F	F
-0.7056562608679293	6.9825803191563871	11.0407582029264013	F	F	F
-0.7124187696122286	4.2167306635848192	15.4009141179224649	T	T	T
-3.1267424153853995	5.5923558153265818	19.7589204208876623	T	T	T
-4.0454627798492222	6.9921131627485487	17.5743152541748024	T	T	T
0.8300507304779470	4.1622897379662023	8.9135372731794220	F	F	F
-1.6423395367524485	5.6022830625817388	13.2221143204608840	F	F	F
-2.3494639853870245	6.8669833935349756	21.0169952551160435	T	T	T
0.8282402647484601	6.8167740087307305	21.8758425090511430	T	T	T
-1.4662743620661185	5.5500313526691967	21.9417599199225393	T	T	T

0.7502178435459466	4.1562078913856766	21.9231162338119070	T	T	T
-1.9816242288234216	4.7116612605301933	21.9641347631205122	T	T	T
0.7529812216169494	6.5233314221048015	22.7943947977984465	T	T	T
0.2682785714597080	4.2945547301175040	22.7549879813096787	T	T	T
-1.9830643442016103	6.2792479746397412	8.8276013437729759	F	F	F
0.2774046270560055	6.6908227065711072	8.0391937587954807	F	F	F
0.7668810467537330	4.4747931255904119	8.0000000000000000	F	F	F
4.8302012138083441	-0.0598626451741637	12.3918657751636392	F	F	F
7.2341173019217448	1.3287808198334001	16.7363282806881735	T	T	T
4.8346750432000203	-0.0580745367475879	18.9161918041684380	T	T	T
7.2356034930344766	1.3276142468898358	10.0985295441362890	F	F	F
4.8301110582525988	2.7176583188924583	14.5561856244294301	F	F	F
4.8637795346750332	-0.0458196655257135	9.7781175373791616	F	F	F
7.2344015332309093	1.3306747828277459	14.0665571956713524	F	F	F
4.8297497580353603	2.7184704073296491	18.4018781467768058	T	T	T
4.8297465637429555	-0.0581836675391766	16.2413945506665875	T	T	T
7.2332044668162645	1.3302519705926044	20.6938462991109269	T	T	T
4.8357587836784308	2.7166585973902686	11.8834768182986377	F	F	F
6.3227927274022786	-0.0557229532918848	11.0348070799988349	F	F	F
8.7073913043724627	1.3302664638227784	15.4001274447179952	T	T	T
6.3189993316318560	2.7149240662459526	19.7605263347910878	T	T	T
5.5664670864059307	1.2184880831617189	17.5763743565881363	T	T	T
7.9714336937132915	2.6640563837800202	8.8712015584813955	F	F	F
5.5687455105299550	3.9930906183199357	13.2250185171475483	F	F	F
4.0841792249349513	1.2288386695443176	11.0371856277262967	F	F	F
6.4970074547492143	2.6049174903475518	15.3991011228151855	T	T	T
4.0998016417677752	3.9998606995920762	19.7541047828348120	T	T	T
8.1661992706971329	-0.0603679293857846	17.5729566469362233	T	T	T
5.7447332033118377	1.2747055185112466	8.8494658732768272	F	F	F
3.3588233710575581	2.7193105234734158	13.2250148374957792	F	F	F
6.5041701284599327	2.8199851124674757	11.0407582029264013	F	F	F
6.4974076197156334	0.0541354568959082	15.4009141179224649	T	T	T
4.0830839739424620	1.4297606086376711	19.7589204208876623	T	T	T
3.1643636094786398	2.8295179560596382	17.5743152541748024	T	T	T
8.0398771198058085	-0.0003054687227085	8.9135372731794220	F	F	F
5.5674868525754135	1.4396878558928281	13.2221143204608840	F	F	F
4.8603624039408375	2.7043881868460646	21.0169952551160435	T	T	T
8.0380666540763226	2.6541788020418196	21.8758425090511430	T	T	T
5.7435520272617433	1.3874361459802860	21.9417599199225393	T	T	T
7.9600442328738090	-0.0063873153032344	21.9231162338119070	T	T	T
5.2282021605044404	0.5490660538412827	21.9641347631205122	T	T	T
7.9628076109448109	2.3607362154158902	22.7943947977984465	T	T	T
7.4781049607875705	0.1319595234285929	22.7549879813096787	T	T	T
5.2267620451262520	2.1166527679508298	8.8276013437729759	F	F	F
7.4872310163838680	2.5282274998821963	8.0391937587954807	F	F	F
7.9767074360815950	0.3121979189015009	8.0000000000000000	F	F	F
2.4269257506990574	4.1027325615147472	12.3918657751636392	F	F	F
4.8308418388124581	5.4913760265223113	16.7363282806881735	T	T	T
2.4313995800907335	4.1045206699413228	18.9161918041684380	T	T	T
4.8323280299251898	5.4902094535787462	10.0985295441362890	F	F	F
2.4268355951433125	6.8802535255813693	14.5561856244294301	F	F	F
2.4605040715657465	4.1167755411631974	9.7781175373791616	F	F	F
4.8311260701216225	5.4932699895166568	14.0665571956713524	F	F	F
2.4264742949260740	6.8810656140185600	18.4018781467768058	T	T	T
2.4264711006336688	4.1044115391497344	16.2413945506665875	T	T	T
4.8299290037069778	5.4928471772815151	20.6938462991109269	T	T	T
2.4324833205691441	6.8792538040791795	11.8834768182986377	F	F	F
3.9195172642929914	4.1068722533970261	11.0348070799988349	F	F	F
6.3041158412631759	5.4928616705116893	15.4001274447179952	T	T	T
3.9157238685225688	6.8775192729348635	19.7605263347910878	T	T	T
3.1631916232966435	5.3810832898506300	17.5763743565881363	T	T	T
5.5681582306040047	6.8266515904689307	8.8712015584813955	F	F	F
3.1654700474206687	8.1556858250088471	13.2250185171475483	F	F	F

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  1.6809037618256641  5.3914338762332283 11.0371856277262967   F   F   F
  4.0937319916399275  6.7675126970364623 15.3991011228151855   T   T   T
  1.6965261786584889  8.1624559062809876 19.7541047828348120   T   T   T
  5.7629238075878462  4.1022272773031263 17.5729566469362233   T   T   T
  3.3414577402025505  5.4373007252001573  8.8494658732768272   F   F   F
  0.9555479079482712  6.8819057301623268 13.2250148374957792   F   F   F
  4.1008946653506460  6.9825803191563871 11.0407582029264013   F   F   F
  4.0941321566063467  4.2167306635848192 15.4009141179224649   T   T   T
  1.6798085108331757  5.5923558153265818 19.7589204208876623   T   T   T
  0.7610881463693528  6.9921131627485487 17.5743152541748024   T   T   T
  5.6366016566965218  4.1622897379662023  8.9135372731794220   F   F   F
  3.1642113894661268  5.6022830625817388 13.2221143204608840   F   F   F
  2.4570869408315508  6.8669833935349756 21.0169952551160435   T   T   T
  5.6347911909670358  6.8167740087307305 21.8758425090511430   T   T   T
  3.3402765641524566  5.5500313526691967 21.9417599199225393   T   T   T
  5.5567687697645223  4.1562078913856766 21.9231162338119070   T   T   T
  2.8249266973951537  4.7116612605301933 21.9641347631205122   T   T   T
  5.5595321478355242  6.5233314221048015 22.7943947977984465   T   T   T
  5.0748294976782837  4.2945547301175040 22.7549879813096787   T   T   T
  2.8234865820169652  6.2792479746397412  8.8276013437729759   F   F   F
  5.0839555532745813  6.6908227065711072  8.0391937587954807   F   F   F
  5.5734319729723083  4.4747931255904119  8.0000000000000000   F   F   F

Metal reference: O-a-Al2O3(0001)/fcc(111)_sqrt13/Ru E_tot= -346.90422298 eV
 D3-zero damping= -13.455925 eV, D3-BJ damping= -16.3495463 eV
Ru
 1.0000000000000000
     9.6131018524371505    0.0000000000000000    0.0000000000000000
    -4.8065509262185726    8.3251904133778201    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000826513396410  0.0000611627174696  8.1577662162144566
  2.5864426983151581  0.6384919669851078  8.1644494024803524
  7.7666900551685263  1.9205916063303354  8.1645047124865808
  0.7398747010818469  2.5588655681741841  8.1644977123994416
  3.3302111474177933  3.2041027686035490  8.1630370905908745
 -1.1099929157854205  4.4863543331104383  8.1627265064661483
  1.4762738425757496  5.1206987502797512  8.1626949740599883
  4.0663676232988166  5.7659368205456332  8.1644395513534853
 -0.3662209267738910  7.0432288367882947  8.1626890527510003
  2.2206039948119449  7.6864853264218604  8.1643858015191526
  8.1360317027188032  0.4271903432608939 10.2746743935190779
  1.1085874662729851  1.0655906280386673 10.2747348746579643
  6.2836480163010506  2.3478291207642972 10.2748597935757466
 -0.7411076848681556  2.9905283871419410 10.2743757365935782
  1.8462439296685527  3.6285766108600050 10.2746995680246602
  0.0000092103435196  5.5501224084072858 10.2748492021362381
  2.5873297237009507  6.1881746065173511 10.2742665790831733
  0.7410253199511938  8.1097879823209471 10.2747015706735301
 -3.3301026759545764  7.8963175169299920 12.3862488169836684
 -0.3667610186832277  1.4930290600322220 12.3862783903154359
  2.2200946156308454  2.1365690988161057 12.3849307582981201
  7.3925273384519388  3.4136908610763674 12.3850539492385359
  0.3663852708824048  4.0570565152918512 12.3862574059209170
  2.9606626539991705  4.6951595896647476 12.3849340642501851
 -1.4762506923497141  5.9794798618487572 12.3863389250924634
  1.1099098245888284  6.6139431956721468 12.3861979316555466
  3.6969435574140115  7.2609187643257389 12.3862372972196848
  6.6528829488256411  0.8542927511143853 12.3849945534322305
  5.1731987450609838  1.2819555957198334  8.1629580373446178
  5.9163683213205189  3.8390617187169647  8.1630518314664844
 -2.9604362335347179  6.4050927668609061  8.1644481171396812
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 -1.8460465710481371  7.4716882974048247 10.2743287363126345
  3.6980597916709383  1.7094967820510352 10.2747952295507829
  4.4380922174913771  4.2679027394400739 10.2748674454067022
 -2.5870354427028053  4.9120780552207295 10.2747304225034313
  5.1751840484890703  6.8323223443902217 10.2747250526018128
  4.0666442603362505  0.2163944678194401 12.3849581777753475
  4.8067571678889465  2.7750218830689124 12.3915656006390620
  5.5469711059246167  5.3342786720518474 12.3848826350172825

Interface: TiO2(110)/fcc(100)_7x1/Au E_tot= -711.88317071 eV
 D3-zero damping= -22.8335101 eV, D3-BJ damping= -26.016285 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Au
 1.0000000000000000
    20.291261973290005 5    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8987517104700005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.2561367997801653
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2  21
Selective dynamics
Cartesian
  0.0000000000000007  1.4493758552350009  9.2861208469999976   F   F   F
  0.0000000000000005  0.0000000000000005  7.9999999999999982   F   F   F
  2.0578045142512513  1.4493758552350009  9.2861208469999976   F   F   F
  3.3818769955483345  0.0000000000000006  9.2861208469999976   F   F   F
  3.3818769955483345  1.4493758552350011 12.5708101129999950   F   F   F
  3.3818769955483345  0.0000000000000007 11.2846892659999956   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416939999988   F   F   F
  4.7059494768454186  1.4493758552350009  9.2861208469999976   F   F   F
  5.4396815097995859  1.4493758552350011 12.5708101129999950   F   F   F
  0.0000000000000008  0.0000000000000008 12.5708101129999950   F   F   F
 20.1543483485979209  1.4493760292194739 15.8632251482045508   T   T   T
 -0.0023725207602867  0.0000001309384258 14.6345775919611096   T   T   T
  3.3818769955483345  0.0000000000000008 13.8569309599999944   F   F   F
  1.3240724812970845  1.4493758552350011 12.5708101129999950   F   F   F
  2.0563774821545797  1.4493758550587454 15.8870004352084457   T   T   T
  3.3090079751350494 -0.0000001008872030 15.9166372333812909   T   T   T
  3.3961843229185229  1.4493758503605128 19.2416063097303258   T   T   T
  3.3964464476752285  0.0000000991413050 17.8710548459675032   T   T   T
 20.2886322289667405  0.0000001533257479 17.2381709410678177   T   T   T
  4.7212778600858574  1.4493760757856373 15.8741279799073336   T   T   T
  5.4987179650568683  1.4493760219720557 19.3537989728039612   T   T   T
  0.0193316039089475 -0.0000000037335203 19.1180521293525416   T   T   T
  3.4066015752527141  0.0000001688559289 20.4450027291612138   T   T   T
  1.3057151003480476  1.4493757796763420 19.3455898870338707   T   T   T
  6.7637539910966691  1.4493758552350009  9.2861208469999976   F   F   F
  6.7637539910966691  0.0000000000000005  7.9999999999999982   F   F   F
  8.8215585053479195  1.4493758552350009  9.2861208469999976   F   F   F
 10.1456309866450027  0.0000000000000006  9.2861208469999976   F   F   F
 10.1456309866450027  1.4493758552350011 12.5708101129999950   F   F   F
 10.1456309866450027  0.0000000000000007 11.2846892659999956   F   F   F
  6.7637539910966691  0.0000000000000006 10.5722416939999988   F   F   F
 11.4697034679420877  1.4493758552350009  9.2861208469999976   F   F   F
 12.2034355008962532  1.4493758552350011 12.5708101129999950   F   F   F
  6.7637539910966691  0.0000000000000008 12.5708101129999950   F   F   F
  6.6327501410403817  1.4493761383747807 15.8539632226539648   T   T   T
  6.7756122691575156  0.0000003416818158 14.6301570829668908   T   T   T
 10.1456309866450027  0.0000000000000008 13.8569309599999944   F   F   F
  8.0878264723937541  1.4493758552350011 12.5708101129999950   F   F   F
  8.8255969249923467  1.4493759337426566 15.9032713730732009   T   T   T
 10.0787367056036050  0.0000003681432326 15.9317728525846416   T   T   T
 10.1702149986393593  1.4493758434326285 19.2746341535101564   T   T   T
 10.1521060028176322 -0.0000001220657945 17.9110426140878474   T   T   T
```

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  6.7633922333350718  0.0000002000781517 17.2288348005793139   T   T   T
 11.4794156861907677  1.4493756989331916 15.8970543818172825   T   T   T
 12.2374722940305443  1.4493755546092870 19.3429453258147568   T   T   T
  6.7822414591466442  0.0000002096774873 19.0980578177106253   T   T   T
 10.1569796657196729 -0.0000000698446697 20.5230681193772746   T   T   T
  8.0752939327555975  1.4493759193823714 19.3390362576531771   T   T   T
 13.5275079821933364  1.4493758552350009  9.2861208469999976   F   F   F
 13.5275079821933364  0.0000000000000005  7.9999999999999982   F   F   F
 15.5853124964445904  1.4493758552350009  9.2861208469999976   F   F   F
 16.9093849777416700  0.0000000000000006  9.2861208469999976   F   F   F
 16.9093849777416700  1.4493758552350011 12.5708101129999950   F   F   F
 16.9093849777416700  0.0000000000000007 11.2846892659999956   F   F   F
 13.5275079821933364  0.0000000000000006 10.5722416939999988   F   F   F
 18.2334574590387568  1.4493758552350009  9.2861208469999976   F   F   F
 18.9671894919929187  1.4493758552350011 12.5708101129999950   F   F   F
 13.5275079821933364  0.0000000000000008 12.5708101129999950   F   F   F
 13.4029772208064415  1.4493756896072139 15.8554581907528132   T   T   T
 13.5179929694364880 -0.0000001356512981 14.6290798173291599   T   T   T
 16.9093849777416700  0.0000000000000008 13.8569309599999944   F   F   F
 14.8515804634904178  1.4493758552350011 12.5708101129999950   F   F   F
 15.5715560647507889  1.4493757926735147 15.8800520829052036   T   T   T
 16.8312185121340789  0.0000000000000009 15.9170184862942978   T   T   T
 16.9483769750118540  1.4493758347295826 19.2397664939527111   T   T   T
 16.9060337934235783 -0.0000001650251737 17.8694808830845950   T   T   T
 13.5297172881251644 -0.0000001527570896 17.2297905336071828   T   T   T
 18.2367091567376320  1.4493758425948247 15.8818836980839926   T   T   T
 19.0087281698317980  1.4493757908505984 19.3498975840326644   T   T   T
 13.5445360740800353 -0.0000005168649802 19.0990272313107674   T   T   T
 16.9045338641775551 -0.0000001600460483 20.4416054124173066   T   T   T
 14.8133463970431691  1.4493754910064780 19.3514711297661890   T   T   T
 -0.0018954063745418 -0.0000001350505541 22.3543007490304291   T   T   T
  1.4182424338679807  1.4493748490479457 24.6281493524755248   T   T   T
 -0.0000747663925147  0.0000001350505541 26.7019641473390834   T   T   T
  2.7463125260718502 -0.0000033375049286 22.5822491236454610   T   T   T
  4.3067036570850048  1.4493745625733727 24.5380277847970198   T   T   T
  2.9288917519834241 -0.0000000212811707 26.6962068660595158   T   T   T
  5.6444132267837608 -0.0000003128215998 22.3812308524541734   T   T   T
  7.2339404512039156  1.4493757201844393 24.3883180547590683   T   T   T
  5.8384769607781939 -0.0000001848437624 26.5047467347834456   T   T   T
  8.3944850873040444  0.0000000000000000 22.2084317984616071   T   T   T
 10.1452922091704316  1.4493758552350002 24.0659453097893596   T   T   T
  8.7634400108519550  0.0000001350505540 26.3422400323811985   T   T   T
 11.9008555223078982  0.0000001350505541 22.2126462168676042   T   T   T
 13.0570032192243684  1.4493756593758667 24.3913191899691846   T   T   T
 11.5263326283484737 -0.0000001958591274 26.3430621088444354   T   T   T
 14.6493321616587533 -0.0000001350505540 22.3824751280569778   T   T   T
 15.9851732270678646  1.4493757476051652 24.5416350481356922   T   T   T
 14.4529416671845485 -0.0000004659602356 26.5056351702262099   T   T   T
 17.5405891841451584  0.0000001958591274 22.5850440330491260   T   T   T
 18.8740191793283998  1.4493758552350002 24.6277420809428769   T   T   T
 17.3649870275672598  0.0000000000000000 26.6977833079787885   T   T   T

Oxide reference: TiO2(110)/fcc(100)_7x1/Au E_tot= -637.90500674 eV
 D3-zero damping= -10.1202152 eV, D3-BJ damping= -14.366457 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O
 1.0000000000000000
    20.2912619732900055    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8987517104700005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6832577396346586
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2
Selective dynamics
```

Cartesian

0.0000000000000007	1.4493758552350009	9.2861208469999994	F	F	F
0.0000000000000005	0.0000000000000005	8.0000000000000000	F	F	F
2.0578045142512513	1.4493758552350009	9.2861208469999994	F	F	F
3.3818769955483345	0.0000000000000006	9.2861208469999994	F	F	F
3.3818769955483345	1.4493758552350011	12.5708101129999967	F	F	F
3.3818769955483345	0.0000000000000007	11.2846892659999973	F	F	F
0.0000000000000007	0.0000000000000006	10.5722416940000006	F	F	F
4.7059494768454186	1.4493758552350009	9.2861208469999994	F	F	F
5.4396815097995859	1.4493758552350011	12.5708101129999967	F	F	F
0.0000000000000008	0.0000000000000008	12.5708101129999967	F	F	F
20.2919636178507794	1.4493758552350011	15.8470979611488012	T	T	T
-0.0001554141282822	0.0000000000000012	14.6301766701886784	T	T	T
3.3818769955483345	0.0000000000000008	13.8569309599999961	F	F	F
1.3240724812970845	1.4493758552350011	12.5708101129999967	F	F	F
2.0394224934623715	1.4493758552350011	15.9005506631595885	T	T	T
3.3832338281490477	0.0000000000000010	16.0180414565624929	T	T	T
3.3819371258055635	1.4493758552350018	19.3851800593860801	T	T	T
3.3791811978019579	0.0000000000000011	17.9176571777052018	T	T	T
20.2911205254446401	0.0000000000000010	17.2223239229013920	T	T	T
4.7272492494758760	1.4493758552350011	15.9027224861546514	T	T	T
5.4978855600395331	1.4493758552350018	19.3948351753822834	T	T	T
-0.0001123915321504	0.0000000000000012	19.0778166424769502	T	T	T
3.3809961243420990	0.0000000000000013	20.5182705588068153	T	T	T
1.2661506235981614	1.4493758552350018	19.3963909612210124	T	T	T
6.7637539910966691	1.4493758552350009	9.2861208469999994	F	F	F
6.7637539910966691	0.0000000000000005	8.0000000000000000	F	F	F
8.8215585053479195	1.4493758552350009	9.2861208469999994	F	F	F
10.1456309866450027	0.0000000000000006	9.2861208469999994	F	F	F
10.1456309866450027	1.4493758552350011	12.5708101129999967	F	F	F
10.1456309866450027	0.0000000000000007	11.2846892659999973	F	F	F
6.7637539910966691	0.0000000000000006	10.5722416940000006	F	F	F
11.4697034679420877	1.4493758552350009	9.2861208469999994	F	F	F
12.2034355008962532	1.4493758552350011	12.5708101129999967	F	F	F
6.7637539910966691	0.0000000000000008	12.5708101129999967	F	F	F
6.7662279032096677	1.4493758552350011	15.8480223523005659	T	T	T
6.7672568209630706	0.0000000000000009	14.6308316383310277	T	T	T
10.1456309866450027	0.0000000000000008	13.8569309599999961	F	F	F
8.0878264723937541	1.4493758552350011	12.5708101129999967	F	F	F
8.8035213103994181	1.4493758552350011	15.9024415133848880	T	T	T
10.1459940416630570	0.0000000000000009	16.0193559983480611	T	T	T
10.1455003839056328	1.4493758552350018	19.3873382264795957	T	T	T
10.1455793531617466	0.0000000000000011	17.9200911934159492	T	T	T
6.7685979616649243	0.0000000000000010	17.2236302257231912	T	T	T
11.4872453169550877	1.4493758552350011	15.9024722215474856	T	T	T
12.2615852517726633	1.4493758552350018	19.3993383254826171	T	T	T
6.7648730854975554	0.0000000000000012	19.0783566943734506	T	T	T
10.1456276457142973	0.0000000000000013	20.5206463170262339	T	T	T
8.0296444896904209	1.4493758552350018	19.3993283982838136	T	T	T
13.5275079821933364	1.4493758552350009	9.2861208469999994	F	F	F
13.5275079821933364	0.0000000000000005	8.0000000000000000	F	F	F
15.5853124964445904	1.4493758552350009	9.2861208469999994	F	F	F
16.9093849777416700	0.0000000000000006	9.2861208469999994	F	F	F
16.9093849777416700	1.4493758552350011	12.5708101129999967	F	F	F
16.9093849777416700	0.0000000000000007	11.2846892659999973	F	F	F
13.5275079821933364	0.0000000000000006	10.5722416940000006	F	F	F
18.2334574590387568	1.4493758552350009	9.2861208469999994	F	F	F
18.9671894919929187	1.4493758552350011	12.5708101129999967	F	F	F
13.5275079821933364	0.0000000000000008	12.5708101129999967	F	F	F
13.5265420574740372	1.4493758552350011	15.8480127954514369	T	T	T
13.5237454746793553	0.0000000000000009	14.6308240820197923	T	T	T
16.9093849777416700	0.0000000000000008	13.8569309599999961	F	F	F
14.8515804634904178	1.4493758552350011	12.5708101129999967	F	F	F

```
 15.5634809004386749  1.4493758552350011 15.9026634169539598   T   T   T
 16.9086951195314050  0.0000000000000009 16.0180261595343509   T   T   T
 16.9089580572994684  1.4493758552350018 19.3851447239571435   T   T   T
 16.9119328753128855  0.0000000000000011 17.9176739366224851   T   T   T
 13.5224496395540683  0.0000000000000010 17.2236164603766078   T   T   T
 18.2512730355831607  1.4493758552350011 15.9006224151129505   T   T   T
 19.0250990677453302  1.4493758552350018 19.3964168538548662   T   T   T
 13.5261803222128645  0.0000000000000011 19.0783532170536958   T   T   T
 16.9102467209103331  0.0000000000000012 20.5183095368619881   T   T   T
 14.7933370627504903  1.4493758552350018 19.3948312260593099   T   T   T

Metal reference: TiO2(110)/fcc(100)_7x1/Au E_tot= -69.94060813 eV
 D3-zero damping= -8.6117002 eV, D3-BJ damping= -8.6879198 eV
Au
 1.0000000000000000
    20.2912619732900055    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8987517104700005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.1817301592405194
  21
Cartesian
 -0.0003457825393010  0.0000000000000000  8.1393930080585370
  1.4467409919203083  1.4493758552350002 10.2241841441184267
 -0.0000912786564196 -0.0000001689775794 12.3076766594506530
  2.8920343725443827 -0.0000001689775794  8.1359877519228654
  4.3460847240873068  1.4493756862574163 10.2192560264035013
  2.8999330885327868  0.0000003379551587 12.3020427299171562
  5.7909530273774319 -0.0000000011325485  8.1303542401266391
  7.2502318526067535  1.4493758552350002 10.2078057594053444
  5.8074741645142476  0.0000003390877072 12.2933037072286258
  8.6962161049353313 -0.0000003379551587  8.1239579584606076
 10.1454667245000465  1.4493760242125842 10.2069912827232923
  8.7015958634977046 -0.0000001689775794 12.2934450917817646
 11.5950778360446805  0.0000001689775794  8.1239788289458499
 13.0408282212090096  1.4493756862574163 10.2076553401882304
 11.5895834723799833  0.0000003379551587 12.2935389960293868
 14.4997988077408042 -0.0000000000000000  8.1302768942293770
 15.9451506499998352  1.4493756862574163 10.2194470251858238
 14.4835424765528220 -0.0000000000000000 12.2934440102863345
 17.3991150919047826 -0.0000000000000000  8.1357525259306005
 18.8438172873271661  1.4493760242125842 10.2242536490847140
 17.3911040296915971 -0.0000000000000000 12.3024572182181551

Interface: TiO2(110)/fcc(100)_7x1/Ag E_tot= -699.77357216 eV
 D3-zero damping= -20.4922045 eV, D3-BJ damping= -25.3159726 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ag
 1.0000000000000000
    20.1636893636500041    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8805270519500006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.2561367997801653
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2  21
Selective dynamics
Cartesian
  0.0000000000000007  1.4402635259750010  9.2861208469999976   F   F   F
  0.0000000000000005  0.0000000000000005  7.9999999999999982   F   F   F
  2.0448669506656265  1.4402635259750010  9.2861208469999976   F   F   F
  3.3606148939416678  0.0000000000000006  9.2861208469999976   F   F   F
  3.3606148939416678  1.4402635259750012 12.5708101129999950   F   F   F
  3.3606148939416678  0.0000000000000007 11.2846892659999956   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416939999988   F   F   F
  4.6763628372177104  1.4402635259750010  9.2861208469999976   F   F   F
  5.4054818446072943  1.4402635259750012 12.5708101129999950   F   F   F
```

0.0000000000000008	0.0000000000000007	12.5708101129999950	F	F	F
20.1636464751982025	1.4402635126623522	15.8691473378407295	T	T	T
0.0000264985237775	0.0000000340904570	14.6330015846483850	T	T	T
3.3606148939416678	0.0000000000000008	13.8569309599999944	F	F	F
1.3157479432760424	1.4402635259750012	12.5708101129999950	F	F	F
2.0262947968416762	1.4402635466802787	15.9145088032465996	T	T	T
3.3607999434221645	0.0000000000000009	15.9301994745426221	T	T	T
3.3503239739203603	1.4402633407678813	19.2940143900874190	T	T	T
3.3633319794946499	-0.0000000780868517	17.9295635195086831	T	T	T
20.1637389590623570	0.0000000151974016	17.2707042190796685	T	T	T
4.6971200889537528	1.4402635645875617	15.9049922526785732	T	T	T
5.4605631880209335	1.4402633825666751	19.4140735684738637	T	T	T
0.0001080358310379	0.0000000000000011	19.1205732511612929	T	T	T
3.4298794115081508	-0.0000000885488067	20.5244463647924746	T	T	T
1.2898805231756620	1.4402634812192596	19.4528034542589694	T	T	T
6.7212297878833356	1.4402635259750010	9.2861208469999976	F	F	F
6.7212297878833356	0.0000000000000005	7.9999999999999982	F	F	F
8.7660967385489617	1.4402635259750010	9.2861208469999976	F	F	F
10.0818446818250020	0.0000000000000006	9.2861208469999976	F	F	F
10.0818446818250020	1.4402635259750012	12.5708101129999950	F	F	F
10.0818446818250020	0.0000000000000007	11.2846892659999956	F	F	F
6.7212297878833356	0.0000000000000006	10.5722416939999988	F	F	F
11.3975926251010442	1.4402635259750010	9.2861208469999976	F	F	F
12.1267116324906290	1.4402635259750012	12.5708101129999950	F	F	F
6.7212297878833356	0.0000000000000007	12.5708101129999950	F	F	F
6.7195371393944265	1.4402634422403655	15.8499173326232690	T	T	T
6.7236575583384637	-0.0000000215225618	14.6172372517419884	T	T	T
10.0818446818250020	0.0000000000000008	13.8569309599999944	F	F	F
8.0369777311593769	1.4402635259750012	12.5708101129999950	F	F	F
8.7488730984709129	1.4402634779905579	15.9015828769404219	T	T	T
10.0818210449729637	0.0000000000000009	15.9092197536913762	T	T	T
10.0819644893384730	1.4402636097096373	19.2673956392325074	T	T	T
10.0819448159544454	0.0000001131614664	17.9217274445073400	T	T	T
6.7243155737934561	-0.0000000844479907	17.2379665485193492	T	T	T
11.4148914265123302	1.4402635127102892	15.9015309527642348	T	T	T
12.1417586719586890	1.4402638312232749	19.3942295429440854	T	T	T
6.7287435481945508	-0.0000001433365523	19.0860309658231557	T	T	T
10.0819110807159529	0.0000000725564670	20.5368305865986081	T	T	T
8.0220993895980026	1.4402635016681276	19.3941775817090409	T	T	T
13.4424595757666694	1.4402635259750010	9.2861208469999976	F	F	F
13.4424595757666694	0.0000000000000005	7.9999999999999982	F	F	F
15.4873265264322981	1.4402635259750010	9.2861208469999976	F	F	F
16.8030744697083385	0.0000000000000006	9.2861208469999976	F	F	F
16.8030744697083385	1.4402635259750012	12.5708101129999950	F	F	F
16.8030744697083385	0.0000000000000007	11.2846892659999956	F	F	F
13.4424595757666694	0.0000000000000006	10.5722416939999988	F	F	F
18.1188224129843789	1.4402635259750010	9.2861208469999976	F	F	F
18.8479414203739637	1.4402635259750012	12.5708101129999950	F	F	F
13.4424595757666694	0.0000000000000007	12.5708101129999950	F	F	F
13.4440530142259167	1.4402636458441227	15.8499139827526268	T	T	T
13.4400777971903960	0.0000000821725729	14.6172728119009498	T	T	T
16.8030744697083385	0.0000000000000008	13.8569309599999944	F	F	F
14.7582075190427080	1.4402635259750012	12.5708101129999950	F	F	F
15.4665835028723997	1.4402635408945386	15.9050027994903012	T	T	T
16.8028553910692757	0.0000001436768785	15.9302409851028060	T	T	T
16.8134876796221455	1.4402635494590232	19.2940931073889104	T	T	T
16.8004747187628674	-0.0000000250917406	17.9295883593692373	T	T	T
13.4394143343731560	0.0000001436768786	17.2379973129864581	T	T	T
18.1374417401419876	1.4402636342857986	15.9145106630023658	T	T	T
18.8739647484377642	1.4402634664141216	19.4528173644872311	T	T	T
13.4351510511331558	0.0000003895589095	19.0860541973101618	T	T	T
16.7339597877756638	0.0000000741477878	20.5244769477324489	T	T	T
14.7032798446407948	1.4402638232452023	19.4140520097443599	T	T	T

```
 -0.0000746068702479 -0.0000000000000000 22.5708478579524510   T   T   T
  1.4349011213484539  1.4402634848542011 24.6769411294145264   T   T   T
 -0.0000060124005953 -0.0000000000000000 26.7106097006514176   T   T   T
  2.7249549346813189 -0.0000000000000000 22.6054538686762889   T   T   T
  4.3015996005752211  1.4402635259750003 24.4910035539962188   T   T   T
  2.9636246941917905  0.0000000000000000 26.6542360510783354   T   T   T
  5.5843747994620339 -0.0000000000000000 22.2582357781526561   T   T   T
  7.1469373594895469  1.4402635259750003 24.2242433681692582   T   T   T
  5.8406122535761344  0.0000000000000000 26.4230027797663745   T   T   T
  8.4075964057719688  0.0000000000000000 22.1465007418363662   T   T   T
 10.0817805583119124  1.4402635259750003 24.0744174193333151   T   T   T
  8.6833713517583728 -0.0000000000000000 26.1985531325969205   T   T   T
 11.7561015559984234  0.0000000411207886 22.1465503010568803   T   T   T
 13.0165976672611947  1.4402635259750003 24.2244227147685933   T   T   T
 11.4800547446669725 -0.0000000000000000 26.1986412221229550   T   T   T
 14.5791965986648915 -0.0000000000000000 22.2584301925049814   T   T   T
 15.8619661341963134  1.4402635259750003 24.4911656474879962   T   T   T
 14.3229292517235347  0.0000000411207886 26.4230816590081936   T   T   T
 17.4386126839072340 -0.0000000000000000 22.6055828504506628   T   T   T
 18.7286972994420182  1.4402635259750003 24.6770282192522927   T   T   T
 17.1999489015642375  0.0000000000000000 26.6543277935974672   T   T   T

Oxide reference: TiO2(110)/fcc(100)_7x1/Ag E_tot= -637.93705497 eV
 D3-zero damping= -10.2180399 eV, D3-BJ damping= -14.5342782 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O
 1.0000000000000000
    20.1636893636500041    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8805270519500006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6832577396346586
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2
Selective dynamics
Cartesian
  0.0000000000000007  1.4402635259750010  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  2.0448669506656265  1.4402635259750010  9.2861208469999994   F   F   F
  3.3606148939416678  0.0000000000000006  9.2861208469999994   F   F   F
  3.3606148939416678  1.4402635259750012 12.5708101129999967   F   F   F
  3.3606148939416678  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416940000006   F   F   F
  4.6763628372177104  1.4402635259750010  9.2861208469999994   F   F   F
  5.4054818446072943  1.4402635259750012 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 20.1649077471775442  1.4402635259750012 15.8537367270233904   T   T   T
 -0.0002039027159999  0.0000000000000011 14.6313355535871565   T   T   T
  3.3606148939416678  0.0000000000000008 13.8569309599999961   F   F   F
  1.3157479432760424  1.4402635259750012 12.5708101129999967   F   F   F
  2.0238131071506436  1.4402635259750012 15.9090050866963111   T   T   T
  3.3622329543415348  0.0000000000000010 16.0334252712640968   T   T   T
  3.3603204346016264  1.4402635259750016 19.4080851462205075   T   T   T
  3.3575686322081761  0.0000000000000011 17.9326275696784556   T   T   T
 20.1634825913712348  0.0000000000000010 17.2353332657079683   T   T   T
  4.7001363536112803  1.4402635259750012 15.9110295314514794   T   T   T
  5.4570472811698565  1.4402635259750016 19.4156117593203170   T   T   T
 -0.0000509259006251  0.0000000000000012 19.0885164474398294   T   T   T
  3.3587146588475636  0.0000000000000012 20.5493586031020961   T   T   T
  1.2628651019216404  1.4402635259750016 19.4171011796459183   T   T   T
  6.7212297878833356  1.4402635259750010  9.2861208469999994   F   F   F
  6.7212297878833356  0.0000000000000005  8.0000000000000000   F   F   F
  8.7660967385489617  1.4402635259750010  9.2861208469999994   F   F   F
 10.0818446818250020  0.0000000000000006  9.2861208469999994   F   F   F
 10.0818446818250020  1.4402635259750012 12.5708101129999967   F   F   F
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 10.0818446818250020  0.0000000000000007 11.2846892659999973   F   F   F
  6.7212297878833356  0.0000000000000006 10.5722416940000006   F   F   F
 11.3975926251010442  1.4402635259750010  9.2861208469999994   F   F   F
 12.1267116324906290  1.4402635259750012 12.5708101129999967   F   F   F
  6.7212297878833356  0.0000000000000007 12.5708101129999967   F   F   F
  6.7236801320869981  1.4402635259750012 15.8535561871824253   T   T   T
  6.7250905154556531  0.0000000000000009 14.6310385707706576   T   T   T
 10.0818446818250020  0.0000000000000008 13.8569309599999961   F   F   F
  8.0369777311593769  1.4402635259750012 12.5708101129999967   F   F   F
  8.7453759800333035  1.4402635259750012 15.9101770010230279   T   T   T
 10.0825499902408868  0.0000000000000009 16.0333333094471051   T   T   T
 10.0817711648896839  1.4402635259750016 19.4087228425012448   T   T   T
 10.0817925613182098  0.0000000000000011 17.9341828624764190   T   T   T
  6.7259973873064833  0.0000000000000010 17.2362319661491341   T   T   T
 11.4177426277581642  1.4402635259750012 15.9102743079080575   T   T   T
 12.1809764862463528  1.4402635259750016 19.4203487734807823   T   T   T
  6.7210255094501923  0.0000000000000011 19.0892158772157643   T   T   T
 10.0817825086584385  0.0000000000000012 20.5501220090377856   T   T   T
  7.9826018356046973  1.4402635259750016 19.4202798837870354   T   T   T
 13.4424595757666694  1.4402635259750010  9.2861208469999994   F   F   F
 13.4424595757666694  0.0000000000000005  8.0000000000000000   F   F   F
 15.4873265264322981  1.4402635259750010  9.2861208469999994   F   F   F
 16.8030744697083385  0.0000000000000006  9.2861208469999994   F   F   F
 16.8030744697083385  1.4402635259750012 12.5708101129999967   F   F   F
 16.8030744697083385  0.0000000000000007 11.2846892659999973   F   F   F
 13.4424595757666694  0.0000000000000006 10.5722416940000006   F   F   F
 18.1188224129843789  1.4402635259750010  9.2861208469999994   F   F   F
 18.8479414203739637  1.4402635259750012 12.5708101129999967   F   F   F
 13.4424595757666694  0.0000000000000007 12.5708101129999967   F   F   F
 13.4423373657299354  1.4402635259750012 15.8535115727618763   T   T   T
 13.4382009710018782  0.0000000000000009 14.6311022541972271   T   T   T
 16.8030744697083385  0.0000000000000008 13.8569309599999961   F   F   F
 14.7582075190427080  1.4402635259750012 12.5708101129999967   F   F   F
 15.4628133219304349  1.4402635259750012 15.9109675147604808   T   T   T
 16.8024557006789870  0.0000000000000009 16.0335151138378578   T   T   T
 16.8033500750266818  1.4402635259750016 19.4081373893718592   T   T   T
 16.8059955308798870  0.0000000000000011 17.9326774629143841   T   T   T
 13.4373146469564304  0.0000000000000010 17.2362820239976955   T   T   T
 18.1391125022535391  1.4402635259750012 15.9091193700329825   T   T   T
 18.9007273648370493  1.4402635259750016 19.4171589792527399   T   T   T
 13.4425281235406207  0.0000000000000011 19.0892872605540092   T   T   T
 16.8048841298747007  0.0000000000000012 20.5494013141633154   T   T   T
 14.7065522513432008  1.4402635259750016 19.4155905471463441   T   T   T

Metal reference: TiO2(110)/fcc(100)_7x1/Ag E_tot= -57.12056413 eV
 D3-zero damping= -6.2835394 eV, D3-BJ damping= -7.9086292 eV
Ag
 1.0000000000000000
    20.1636893636500041    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8805270519500006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.1817301592405194
  21
Cartesian
 -0.0001507231637545 -0.0000000000000000  8.1604663196346436
  1.4400072631989538  1.4402635259750003 10.2286751372655136
 -0.0002935584976699 -0.0000000000000000 12.2969841242393070
  2.8782370401177850 -0.0000000000000000  8.1546684579396498
  4.3178100503420458  1.4402635259750003 10.2188712539316189
  2.8848778521842138  0.0000000000000000 12.2926378603912596
  5.7555570776890344 -0.0000000000000000  8.1422021944385019
  7.1992963578601179  1.4402635259750003 10.2063399997341495
  5.7658688354811689  0.0000000000000000 12.2808500840810044
  8.6392382123844218  0.0000001267343649  8.1360126069474870
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 10.0818937876617305  1.4402635259750003 10.2000863612370267
  8.6436636089971159  0.0000001267343649 12.2696193341712725
 11.5243689071773261 -0.0000000000000000  8.1361201732359003
 12.9642539650663409  1.4402635259750003 10.2061600558261816
 11.5199642638550834  0.0000001267343649 12.2695468427065180
 14.4078007774242014  0.0000000000000000  8.1417913940132358
 15.8456079283954008  1.4402635259750003 10.2184327238217865
 14.3975740471222906 -0.0000000000000000 12.2806764460200508
 17.2851417707076997 -0.0000001267343649  8.1542461162814028
 18.7233261495866756  1.4402635259750003 10.2285001120720853
 17.2783467551057299 -0.0000001267343649 12.2923130907937281

Interface: TiO2(110)/fcc(100)_7x1/Pt E_tot= -763.08250862 eV
 D3-zero damping= -24.9024882 eV, D3-BJ damping= -29.2261766 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Pt
 1.0000000000000000
    19.3931735579400026    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7704533654200003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.2561367997801653
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2  21
Selective dynamics
Cartesian
  0.0000000000000006  1.3852266827100008  9.2861208469999976   F   F   F
  0.0000000000000005  0.0000000000000005  7.9999999999999982   F   F   F
  1.9667263744225560  1.3852266827100008  9.2861208469999976   F   F   F
  3.2321955929900006  0.0000000000000005  9.2861208469999976   F   F   F
  3.2321955929900006  1.3852266827100010 12.5708101129999950   F   F   F
  3.2321955929900006  0.0000000000000006 11.2846892659999956   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416939999988   F   F   F
  4.4976648115574465  1.3852266827100008  9.2861208469999976   F   F   F
  5.1989219674125566  1.3852266827100010 12.5708101129999950   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999950   F   F   F
 19.3932186929012573  1.3852266827100010 15.9897817634142925   T   T   T
  0.0000309124859959  0.0000000000000007 14.6135701552650623   T   T   T
  3.2321955929900006  0.0000000000000008 13.8569309599999944   F   F   F
  1.2654692185674457  1.3852266827100010 12.5708101129999950   F   F   F
  1.9723060914958925  1.3852267041257051 15.9079501980776836   T   T   T
  3.2323951521095831  0.0000000000000009 15.9000177585309235   T   T   T
  3.2182071773640533  1.3852267920018906 19.2283454238526446   T   T   T
  3.3308250855220378  0.0000000987832901 17.8761529721305763   T   T   T
 19.3932032009599808 -0.0000000339616587 17.2949891778084215   T   T   T
  4.5575723240077783  1.3852266585607189 15.8528486574725349   T   T   T
  5.2183666705589804  1.3852267636564266 19.5007309519038969   T   T   T
 -0.0000244859847199  0.0000000000000011 19.5854743861334413   T   T   T
  3.2385835341577187  0.0000000770389670 20.5350564865441960   T   T   T
  1.2852820492344772  1.3852266827100015 19.3261156672973229   T   T   T
  6.4643911859800012  1.3852266827100008  9.2861208469999976   F   F   F
  6.4643911859800012  0.0000000000000005  7.9999999999999982   F   F   F
  8.4311175604025568  1.3852266827100008  9.2861208469999976   F   F   F
  9.6965867789700013  0.0000000000000005  9.2861208469999976   F   F   F
  9.6965867789700013  1.3852266827100010 12.5708101129999950   F   F   F
  9.6965867789700013  0.0000000000000006 11.2846892659999956   F   F   F
  6.4643911859800012  0.0000000000000006 10.5722416939999988   F   F   F
 10.9620559975374459  1.3852266827100008  9.2861208469999976   F   F   F
 11.6633131533925578  1.3852266827100010 12.5708101129999950   F   F   F
  6.4643911859800012  0.0000000000000007 12.5708101129999950   F   F   F
  6.4553663195070445  1.3852266827100010 15.8991581904064638   T   T   T
  6.5184712957835789  0.0000000000000009 14.6186387565073446   T   T   T
  9.6965867789700013  0.0000000000000008 13.8569309599999944   F   F   F
  7.7298604045474466  1.3852266827100010 12.5708101129999950   F   F   F
  8.4070590892162027  1.3852266827100010 15.9701393704788526   T   T   T
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  9.6966448174805357  0.0000000000000009 15.9867801431947747   T   T   T
  9.6966575530490928  1.3852266827100015 19.3848713969121675   T   T   T
  9.6966801198693524  0.0000000279131297 18.0110949306646049   T   T   T
  6.4594960456778843 -0.0000000039226847 17.3205490410767666   T   T   T
 10.9861986428017318  1.3852266827100010 15.9701247196004896   T   T   T
 11.6529581930549870  1.3852268040701659 19.5128752696556091   T   T   T
  6.4626418272716606  0.0000000840356821 19.1887734882648360   T   T   T
  9.6966419693714165 -0.0000000059577505 20.7913878893592106   T   T   T
  7.7403801921588604  1.3852267274107708 19.5127941311132389   T   T   T
 12.9287823719600006  1.3852266827100008  9.2861208469999976   F   F   F
 12.9287823719600006  0.0000000000000005  7.9999999999999982   F   F   F
 14.8955087463825588  1.3852266827100008  9.2861208469999976   F   F   F
 16.1609779649499998  0.0000000000000005  9.2861208469999976   F   F   F
 16.1609779649499998  1.3852266827100010 12.5708101129999950   F   F   F
 16.1609779649499998  0.0000000000000006 11.2846892659999956   F   F   F
 12.9287823719600006  0.0000000000000006 10.5722416939999988   F   F   F
 17.4264471835174461  1.3852266827100008  9.2861208469999976   F   F   F
 18.1277043393725563  1.3852266827100010 12.5708101129999950   F   F   F
 12.9287823719600006  0.0000000000000007 12.5708101129999950   F   F   F
 12.9379201545199987  1.3852266827100010 15.8991623859845941   T   T   T
 12.8747492665327758 -0.0000000178545798 14.6186116856079309   T   T   T
 16.1609779649499998  0.0000000000000008 13.8569309599999944   F   F   F
 14.1942515905274433  1.3852266827100010 12.5708101129999950   F   F   F
 14.8356703719888614  1.3852266446796662 15.8527787592669238   T   T   T
 16.1608658398204739 -0.0000000279131278 15.8999725061467760   T   T   T
 16.1749943224288764  1.3852265392230381 19.2282725473844849   T   T   T
 16.0623815715244653 -0.0000001045804663 17.8760341003963603   T   T   T
 12.9337944851386624 -0.0000000100253384 17.3205476760522856   T   T   T
 17.4209592172908856  1.3852266721424429 15.9078926552407491   T   T   T
 18.1079738456937100  1.3852266297991749 19.3259234716642148   T   T   T
 12.9307143834618881  0.0000001472054568 19.1887625843987024   T   T   T
 16.1547933725955453 -0.0000000629129388 20.5349552276673073   T   T   T
 14.1749232282520747  1.3852267708172741 19.5007592622930979   T   T   T
 -0.0004238162170286 -0.0000000000000000 22.1228057842992172   T   T   T
  1.3501171866344512  1.3852265839267133 24.3810228245471770   T   T   T
 -0.0002502433871772 -0.0000001434869628 26.3263472267922332   T   T   T
  2.6525570986007856  0.0000000987832891 22.4623295981176376   T   T   T
  4.1261173147532251  1.3852266827100002 24.4092152349337610   T   T   T
  2.7750269770969123 -0.0000001434869628 26.3557923352646704   T   T   T
  5.5077487835340122 -0.0000000000000000 22.4433422571883057   T   T   T
  6.9127315662805255  1.3852267814932870 24.3811700621723766   T   T   T
  5.5518483885696988  0.0000000000000000 26.3338563417015763   T   T   T
  8.1780612453703547 -0.0000000987832891 22.3929308421160229   T   T   T
  9.6966256601192597  1.3852266827100002 24.2934042773094205   T   T   T
  8.3317795151949632  0.0000001434869628 26.2757076869148989   T   T   T
 11.2149518365405374 -0.0000000447036737 22.3929686523198583   T   T   T
 12.4802050794788055  1.3852265839267133 24.3812665708028042   T   T   T
 11.0609751857510350  0.0000000987832891 26.2758169316021579   T   T   T
 13.8852873248385897 -0.0000001975665783 22.4434760202013983   T   T   T
 15.2668244527377226  1.3852266827100002 24.4095598244724599   T   T   T
 13.8410300958186134 -0.0000000447036737 26.3339312910936165   T   T   T
 16.7399335169870156  0.0000000987832891 22.4626754144968857   T   T   T
 18.0427270375838269  1.3852265839267133 24.3810303610828711   T   T   T
 16.6179882884807846  0.0000000987832891 26.3558538093899841   T   T   T

Oxide reference: TiO2(110)/fcc(100)_7x1/Pt E_tot= -632.69144821 eV
 D3-zero damping= -10.8351544 eV, D3-BJ damping= -15.58687 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O
 1.0000000000000000
    19.3931735579400026    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7704533654200003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6832577396346586
```

```
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.3852266827100008  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.9667263744225560  1.3852266827100008  9.2861208469999994   F   F   F
  3.2321955929900006  0.0000000000000005  9.2861208469999994   F   F   F
  3.2321955929900006  1.3852266827100010 12.5708101129999967   F   F   F
  3.2321955929900006  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.4976648115574465  1.3852266827100008  9.2861208469999994   F   F   F
  5.1989219674125566  1.3852266827100010 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 19.3931717466315057  1.3852266827100010 15.8839229573264351   T   T   T
 -0.0000108846375786  0.0000000000000012 14.6339259419319045   T   T   T
  3.2321955929900006  0.0000000000000008 13.8569309599999961   F   F   F
  1.2654692185674457  1.3852266827100010 12.5708101129999967   F   F   F
  1.9349498613838523  1.3852266827100010 15.9675896806297732   T   T   T
  3.2321862706045565  0.0000000000000009 16.1641550121554118   T   T   T
  3.2321497788150730  1.3852266827100015 19.5823073511314121   T   T   T
  3.2321319053231012  0.0000000000000010 18.0550926419390514   T   T   T
 19.3931940113372612  0.0000000000000010 17.3126184403490946   T   T   T
  4.5294390957801651  1.3852266827100010 15.9676448049578941   T   T   T
  5.2314872702618169  1.3852266827100015 19.5709269874355947   T   T   T
 -0.0000336083307365  0.0000000000000011 19.1510174952176335   T   T   T
  3.2321888427322434  0.0000000000000012 20.7714705223368803   T   T   T
  1.2327947817533378  1.3852266827100015 19.5710341215696495   T   T   T
  6.4643911859800012  1.3852266827100008  9.2861208469999994   F   F   F
  6.4643911859800012  0.0000000000000005  8.0000000000000000   F   F   F
  8.4311175604025568  1.3852266827100008  9.2861208469999994   F   F   F
  9.6965867789700013  0.0000000000000005  9.2861208469999994   F   F   F
  9.6965867789700013  1.3852266827100010 12.5708101129999967   F   F   F
  9.6965867789700013  0.0000000000000006 11.2846892659999973   F   F   F
  6.4643911859800012  0.0000000000000006 10.5722416940000006   F   F   F
 10.9620559975374459  1.3852266827100008  9.2861208469999994   F   F   F
 11.6633131533925578  1.3852266827100010 12.5708101129999967   F   F   F
  6.4643911859800012  0.0000000000000007 12.5708101129999967   F   F   F
  6.4643893424542611  1.3852266827100010 15.8839230175876462   T   T   T
  6.4643801797025828  0.0000000000000009 14.6339260029987859   T   T   T
  9.6965867789700013  0.0000000000000008 13.8569309599999961   F   F   F
  7.7298604045474466  1.3852266827100010 12.5708101129999967   F   F   F
  8.3993409928770824  1.3852266827100010 15.9675896676737743   T   T   T
  9.6965774155622508  0.0000000000000009 16.1641548245452249   T   T   T
  9.6965409531086966  1.3852266827100015 19.5823071687033234   T   T   T
  9.6965230864352279  0.0000000000000010 18.0550924767528294   T   T   T
  6.4644115471735057  0.0000000000000010 17.3126186059092468   T   T   T
 10.9938302280438656  1.3852266827100010 15.9676446955376345   T   T   T
 11.6958784208252080  1.3852266827100015 19.5709268177106139   T   T   T
  6.4643575636171020  0.0000000000000011 19.1510176473558005   T   T   T
  9.6965800571133656  0.0000000000000012 20.7714703379364920   T   T   T
  7.6971859788311265  1.3852266827100015 19.5710341764836215   T   T   T
 12.9287823719600006  1.3852266827100008  9.2861208469999994   F   F   F
 12.9287823719600006  0.0000000000000005  8.0000000000000000   F   F   F
 14.8955087463825588  1.3852266827100008  9.2861208469999994   F   F   F
 16.1609779649499998  0.0000000000000005  9.2861208469999994   F   F   F
 16.1609779649499998  1.3852266827100010 12.5708101129999967   F   F   F
 16.1609779649499998  0.0000000000000006 11.2846892659999973   F   F   F
 12.9287823719600006  0.0000000000000006 10.5722416940000006   F   F   F
 17.4264471835174461  1.3852266827100008  9.2861208469999994   F   F   F
 18.1277043393725563  1.3852266827100010 12.5708101129999967   F   F   F
 12.9287823719600006  0.0000000000000007 12.5708101129999967   F   F   F
 12.9287805367939139  1.3852266827100010 15.8839229466908645   T   T   T
```

```
 12.9287713507534985  0.0000000000000009 14.6339259345258075   T   T   T
 16.1609779649499998  0.0000000000000008 13.8569309599999961   F   F   F
 14.1942515905274433  1.3852266827100010 12.5708101129999967   F   F   F
 14.8637321814771859  1.3852266827100010 15.9675894349825622   T   T   T
 16.1609686398947368  0.0000000000000009 16.1641544958081340   T   T   T
 16.1609321304313127  1.3852266827100015 19.5823068058636913   T   T   T
 16.1609142502392373  0.0000000000000010 18.0550922090245116   T   T   T
 12.9288027636319036  0.0000000000000010 17.3126184610051261   T   T   T
 17.4582214886081211  1.3852266827100010 15.9676446006663912   T   T   T
 18.1602696573845961  1.3852266827100015 19.5709266551794663   T   T   T
 12.9287486954873145  0.0000000000000011 19.1510175343642146   T   T   T
 16.1609712437028890  0.0000000000000012 20.7714699737416559   T   T   T
 14.1615771124244159  1.3852266827100015 19.5710339795207311   T   T   T

Metal reference: TiO2(110)/fcc(100)_7x1/Pt E_tot= -125.45166736 eV
 D3-zero damping= -9.6401945 eV, D3-BJ damping= -10.1010972 eV
Pt
 1.0000000000000000
    19.3931735579400026    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7704533654200003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.1817301592405194
  21
Cartesian
 -0.0001121685329791 -0.0000000000000001  8.2856722821334081
  1.3856027617728310  1.3852266827100002 10.2236797721604304
 -0.0003402134307043 -0.0000000000000000 12.1617949468284667
  2.7700204820388263  0.0000000000000000  8.2847166131940515
  4.1578457448955017  1.3852266827100002 10.2212535292868587
  2.7715367035544984  0.0000000000000000 12.1619922054771088
  5.5375026770596625 -0.0000000000000000  8.2732072720333960
  6.9253035753812568  1.3852266827100002 10.2078599121976339
  5.5460538684778520  0.0000000000000000 12.1546430763154980
  8.3086546985499403  0.0000000000000000  8.2645906051256581
  9.6965510547840097  1.3852266827100002 10.1994002117069087
  8.3143138587654111 -0.0000000000000000 12.1424327862468964
 11.0844314297000377 -0.0000000000000000  8.2643835907599232
 12.4676437586546278  1.3852266827100002 10.2079003889258626
 11.0786920686717707  0.0000000000000000 12.1424529392751559
 13.8553462979890831 -0.0000000000000000  8.2731389721256363
 15.2350632897762832  1.3852266827100002 10.2210749968073582
 13.8469871896194689 -0.0000000000000000 12.1545996394560945
 16.6229377723629526 -0.0000000000000000  8.2847458744822102
 18.0072978469366305  1.3852266827100002 10.2236494661761910
 16.6212591273924524  0.0000000000000000 12.1620115500364729

Interface: TiO2(110)/fcc(100)_7x1/Pd E_tot= -742.08945616 eV
 D3-zero damping= -22.4500364 eV, D3-BJ damping= -27.7829056 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Pd
 1.0000000000000000
    19.2358686233000036    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7479812319000003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.2561367997801653
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2  21
Selective dynamics
Cartesian
  0.0000000000000006  1.3739906159500008  9.2861208469999976   F   F   F
  0.0000000000000005  0.0000000000000005  7.9999999999999982   F   F   F
  1.9507735566509317  1.3739906159500008  9.2861208469999976   F   F   F
  3.2059781038833344  0.0000000000000005  9.2861208469999976   F   F   F
  3.2059781038833344  1.3739906159500010 12.5708101129999950   F   F   F
  3.2059781038833344  0.0000000000000006 11.2846892659999956   F   F   F
```

0.0000000000000006	0.0000000000000006	10.5722416939999988	F	F	F
4.4611826511157373	1.3739906159500008	9.2861208469999976	F	F	F
5.1567516605342654	1.3739906159500010	12.5708101129999950	F	F	F
0.0000000000000008	0.0000000000000007	12.5708101129999950	F	F	F
19.2359131432702668	1.3739906159500010	15.9182651939877537	T	T	T
0.0000683397075586	-0.0000000494178478	14.6241852194216033	T	T	T
3.2059781038833344	0.0000000000000008	13.8569309599999944	F	F	F
1.2552045472324036	1.3739906159500010	12.5708101129999950	F	F	F
1.9124577103733003	1.3739906205905918	15.9383065408336240	T	T	T
3.2046821601377795	0.0000000000000008	16.0131936231606176	T	T	T
3.2035185813867857	1.3739906159500015	19.4034218327040264	T	T	T
3.1925303066209278	-0.0000000169559089	17.9806131035452914	T	T	T
19.2358613283783022	-0.0000000620073455	17.3674475202511900	T	T	T
4.4997515585874437	1.3739906083105804	15.9395498025014106	T	T	T
5.1760564223799319	1.3739906542777773	19.5338454981236893	T	T	T
0.0000767217478325	0.0000000000000011	19.2258686262955969	T	T	T
3.2981698481855704	-0.0000000125110107	20.7004287309626243	T	T	T
1.2505012869560816	1.3739906141869094	19.6333068930591637	T	T	T
6.4119562077666687	1.3739906159500008	9.2861208469999976	F	F	F
6.4119562077666687	0.0000000000000005	7.9999999999999982	F	F	F
8.3627297644175993	1.3739906159500008	9.2861208469999976	F	F	F
9.6179343116500018	0.0000000000000005	9.2861208469999976	F	F	F
9.6179343116500018	1.3739906159500010	12.5708101129999950	F	F	F
9.6179343116500018	0.0000000000000006	11.2846892659999956	F	F	F
6.4119562077666687	0.0000000000000006	10.5722416939999988	F	F	F
10.8731388588824043	1.3739906159500008	9.2861208469999976	F	F	F
11.5687078683009332	1.3739906159500010	12.5708101129999950	F	F	F
6.4119562077666687	0.0000000000000007	12.5708101129999950	F	F	F
6.4115595665261980	1.3739906150202410	15.8886822901890259	T	T	T
6.4115134707520465	-0.0000000438837528	14.6018332873328056	T	T	T
9.6179343116500018	0.0000000000000008	13.8569309599999944	F	F	F
7.6671607549990712	1.3739906159500010	12.5708101129999950	F	F	F
8.3257669495941542	1.3739905983443546	15.9346433587736165	T	T	T
9.6180075736253539	0.0000000000000009	16.0128092338450720	T	T	T
9.6180932377875017	1.3739906159500015	19.4088522115713431	T	T	T
9.6180916193534038	-0.0000000188552077	17.9919886063857177	T	T	T
6.4188017037555687	-0.0000000042671051	17.3191648780880989	T	T	T
10.9102240495587299	1.3739905803899584	15.9345333043869921	T	T	T
11.5680969984091906	1.3739906166746121	19.5639984723668086	T	T	T
6.4212552634022231	0.0000000850376118	19.1670134605217193	T	T	T
9.6179395037723676	0.0000000345504940	20.7575528145196522	T	T	T
7.6680426854610380	1.3739906400914492	19.5638353906648632	T	T	T
12.8239124155333357	1.3739906159500008	9.2861208469999976	F	F	F
12.8239124155333357	0.0000000000000005	7.9999999999999982	F	F	F
14.7746859721842689	1.3739906159500008	9.2861208469999976	F	F	F
16.0298905194166679	0.0000000000000005	9.2861208469999976	F	F	F
16.0298905194166679	1.3739906159500010	12.5708101129999950	F	F	F
16.0298905194166679	0.0000000000000006	11.2846892659999956	F	F	F
12.8239124155333357	0.0000000000000006	10.5722416939999988	F	F	F
17.2850950666490739	1.3739906159500008	9.2861208469999976	F	F	F
17.9806640760675975	1.3739906159500010	12.5708101129999950	F	F	F
12.8239124155333357	0.0000000000000007	12.5708101129999950	F	F	F
12.8244448041192172	1.3739907428722598	15.8887164383493751	T	T	T
12.8244765720918235	0.0000000682771556	14.6018947479089167	T	T	T
16.0298905194166679	0.0000000000000008	13.8569309599999944	F	F	F
14.0791169627657347	1.3739906159500010	12.5708101129999950	F	F	F
14.7362280163174422	1.3739904380129806	15.9397166126203640	T	T	T
16.0312942176958124	-0.0000002232110211	16.0136951784134176	T	T	T
16.0325877041350218	1.3739903536373521	19.4036646441334533	T	T	T
16.0435856399196020	-0.0000001211892759	17.9808028679177809	T	T	T
12.8171604568846380	0.0000000000000010	17.3192115189909650	T	T	T
17.3234765071049530	1.3739904331252197	15.9382415067053280	T	T	T
17.9854847292204489	1.3739906407633340	19.6334589828278965	T	T	T

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 12.8148904364185210  0.0000000160003370 19.1670635682944059   T   T   T
 15.9378896006878374 -0.0000001276094964 20.7005286242318576   T   T   T
 14.0600260659321723  1.3739905839478996 19.5340070272862789   T   T   T
 -0.0001410128513433 -0.0000000000000000 22.5334804246022102   T   T   T
  1.3541235597669650  1.3739906159500002 24.5756015860015467   T   T   T
 -0.0000417357020048 -0.0000000000000000 26.5401830310713365   T   T   T
  2.6224598446654861 -0.0000000000000000 22.6236564670106866   T   T   T
  4.1309120801436041  1.3739906159500002 24.4689286236181225   T   T   T
  2.7941229829096379 -0.0000000000000000 26.4624698240388305   T   T   T
  5.4085452887049268 -0.0000000000000000 22.3560389350991215   T   T   T
  6.8300796256150438  1.3739906159500002 24.3010299397321567   T   T   T
  5.5618221967305042  0.0000000000000000 26.3580153750011021   T   T   T
  8.1133237993232488  0.0000000000000000 22.3355101968080980   T   T   T
  9.6176180749355691  1.3739906159500002 24.2425504583833096   T   T   T
  8.2619263174741526 -0.0000000000000000 26.2086555354045174   T   T   T
 11.1221966538165358 -0.0000000000000000 22.3356200096591841   T   T   T
 12.4052789838886124  1.3739906159500002 24.3009315121756586   T   T   T
 10.9736320784241208  0.0000000000000000 26.2087312760598152   T   T   T
 13.8272532193307889  0.0000000000000000 22.3564031841548356   T   T   T
 15.1048280537622528  1.3739906159500002 24.4691369707443229   T   T   T
 13.6737605495386170 -0.0000000000000000 26.3577605055157171   T   T   T
 16.6131236863236147 -0.0000000855423678 22.6239463179637852   T   T   T
 17.8813097931163227  1.3739907014923654 24.5755917000621018   T   T   T
 16.4412663160692034 -0.0000000000000000 26.4627211759055001   T   T   T

Oxide reference: TiO2(110)/fcc(100)_7x1/Pd E_tot= -630.28450832 eV
 D3-zero damping= -10.9607439 eV, D3-BJ damping= -15.796621 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O
 1.0000000000000000
    19.2358686233000036    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7479812319000003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6832577396346586
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.3739906159500008  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.9507735566509317  1.3739906159500008  9.2861208469999994   F   F   F
  3.2059781038833344  0.0000000000000005  9.2861208469999994   F   F   F
  3.2059781038833344  1.3739906159500010 12.5708101129999967   F   F   F
  3.2059781038833344  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.4611826511157373  1.3739906159500008  9.2861208469999994   F   F   F
  5.1567516605342654  1.3739906159500010 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 19.2358375883328669  1.3739906159500010 15.8932600913198936   T   T   T
 -0.0000234119269945  0.0000000000000012 14.6379546407900083   T   T   T
  3.2059781038833344  0.0000000000000008 13.8569309599999961   F   F   F
  1.2552045472324036  1.3739906159500010 12.5708101129999967   F   F   F
  1.9189197783549605  1.3739906159500010 15.9847294767801582   T   T   T
  3.2059478563853925  0.0000000000000010 16.2106014647241636   T   T   T
  3.2059597897376491  1.3739906159500015 19.6370728752210795   T   T   T
  3.2059421677137907  0.0000000000000010 18.0968342025332412   T   T   T
 19.2358652143330602  0.0000000000000010 17.3355695966700587   T   T   T
  4.4929878312003755  1.3739906159500010 15.9847431756987852   T   T   T
  5.1880439729890711  1.3739906159500015 19.6209449365748689   T   T   T
 -0.0000008980360059  0.0000000000000011 19.1712928921497330   T   T   T
  3.2060004004744034  0.0000000000000012 20.8346075875752774   T   T   T
  1.2238868889218224  1.3739906159500015 19.6210411138286567   T   T   T
  6.4119562077666687  1.3739906159500008  9.2861208469999994   F   F   F
  6.4119562077666687  0.0000000000000005  8.0000000000000000   F   F   F
```

```
  8.3627297644175993  1.3739906159500008  9.2861208469999994   F   F   F
  9.6179343116500018  0.0000000000000005  9.2861208469999994   F   F   F
  9.6179343116500018  1.3739906159500010 12.5708101129999967   F   F   F
  9.6179343116500018  0.0000000000000006 11.2846892659999973   F   F   F
  6.4119562077666687  0.0000000000000006 10.5722416940000006   F   F   F
 10.8731388588824043  1.3739906159500008  9.2861208469999994   F   F   F
 11.5687078683009332  1.3739906159500010 12.5708101129999967   F   F   F
  6.4119562077666687  0.0000000000000007 12.5708101129999967   F   F   F
  6.4119250118711388  1.3739906159500010 15.8932601751833058   T   T   T
  6.4119324774353812  0.0000000000000009 14.6379547307622726   T   T   T
  9.6179343116500018  0.0000000000000008 13.8569309599999961   F   F   F
  7.6671607549990712  1.3739906159500010 12.5708101129999967   F   F   F
  8.3308758958615794  1.3739906159500010 15.9847290946491345   T   T   T
  9.6179040316405047  0.0000000000000009 16.2106006276929158   T   T   T
  9.6179160331612064  1.3739906159500015 19.6370719751724749   T   T   T
  9.6178984088382720  0.0000000000000010 18.0968335165591476   T   T   T
  6.4119529104734925  0.0000000000000010 17.3355697376775666   T   T   T
 10.9049440703973026  1.3739906159500010 15.9847426427772916   T   T   T
 11.6000002689914936  1.3739906159500015 19.6209446440609625   T   T   T
  6.4119553282413353  0.0000000000000011 19.1712930335780634   T   T   T
  9.6179566844665043  0.0000000000000012 20.8346067293145580   T   T   T
  7.6358430729769537  1.3739906159500015 19.6210410509186630   T   T   T
 12.8239124155333357  1.3739906159500008  9.2861208469999994   F   F   F
 12.8239124155333357  0.0000000000000005  8.0000000000000000   F   F   F
 14.7746859721842689  1.3739906159500008  9.2861208469999994   F   F   F
 16.0298905194166679  0.0000000000000005  9.2861208469999994   F   F   F
 16.0298905194166679  1.3739906159500010 12.5708101129999967   F   F   F
 16.0298905194166679  0.0000000000000006 11.2846892659999973   F   F   F
 12.8239124155333357  0.0000000000000006 10.5722416940000006   F   F   F
 17.2850950666490739  1.3739906159500008  9.2861208469999994   F   F   F
 17.9806640760675975  1.3739906159500010 12.5708101129999967   F   F   F
 12.8239124155333357  0.0000000000000007 12.5708101129999967   F   F   F
 12.8238813132923539  1.3739906159500010 15.8932600118831306   T   T   T
 12.8238889187872651  0.0000000000000009 14.6379545993910121   T   T   T
 16.0298905194166679  0.0000000000000008 13.8569309599999961   F   F   F
 14.0791169627657347  1.3739906159500010 12.5708101129999967   F   F   F
 14.7428321511330704  1.3739906159500010 15.9847291801260862   T   T   T
 16.0298603099913635  0.0000000000000009 16.2106006816983310   T   T   T
 16.0298721738229126  1.3739906159500015 19.6370720453548167   T   T   T
 16.0298545656067617  0.0000000000000010 18.0968335624417982   T   T   T
 12.8239089880493697  0.0000000000000010 17.3355694904204718   T   T   T
 17.3169003261676906  1.3739906159500010 15.9847427189534415   T   T   T
 18.0119564501016391  1.3739906159500015 19.6209446374614345   T   T   T
 12.8239115330964086  0.0000000000000011 19.1712928018403623   T   T   T
 16.0299128655937153  0.0000000000000012 20.8346068003575837   T   T   T
 14.0477992864901040  1.3739906159500015 19.6210409450857668   T   T   T

Metal reference: TiO2(110)/fcc(100)_7x1/Pd E_tot= -106.61084692 eV
 D3-zero damping= -7.1309733 eV, D3-BJ damping= -8.7126362 eV
Pd
 1.0000000000000000
    19.2358686233000036    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7479812319000003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.1817301592405194
  21
Cartesian
 -0.0000335211984611  0.0000000000000000  8.2677410764945503
  1.3725036816973073  1.3739906159500002 10.2250633388904060
 -0.0001314115993165 -0.0000000000000000 12.1833933639788263
  2.7435172067950653 -0.0000000000000000  8.2641541379584833
  4.1207511558141938  1.3739906159500002 10.2161170757686026
  2.7492760106147300  0.0000000000000000 12.1767414393384019
  5.4927141784344933 -0.0000000000000000  8.2549126534542481
```

```
  6.8684826098367706  1.3739906159500002 10.2097520999787772
  5.4966737751294072  0.0000000000000000 12.1682392826601617
  8.2411984248787888  0.0000000000000000  8.2532499568578892
  9.6178297364923697  1.3739906159500002 10.2047687662882005
  8.2449864670051678 -0.0000000000000000 12.1618830162711671
 10.9943235994340096  0.0000000000000000  8.2531633800489193
 12.3671309023120788  1.3739906159500002 10.2096518983071416
 10.9907138566789619  0.0000000000000000 12.1618794023816790
 13.7427742023221189  0.0000000000000000  8.2547264710389250
 15.1148877838324651  1.3739906159500002 10.2159774220874056
 13.7389643462616018 -0.0000000000000000 12.1681796518859269
 16.4920986489876320 -0.0000000000000000  8.2640197823783677
 17.8631866885193844  1.3739906159500002 10.2250567739255604
 16.4863670961980269  0.0000000000000000 12.1765297022929406

Interface: TiO2(110)/fcc(100)_7x1/Ir E_tot= -807.52003039 eV
 D3-zero damping= -23.8566203 eV, D3-BJ damping= -28.9598739 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ir
 1.0000000000000000
    19.0054425018500055    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7150632145500007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.2561367997801653
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2  21
Selective dynamics
Cartesian
  0.0000000000000006  1.3575316072750010  9.2861208469999976   F   F   F
  0.0000000000000005  0.0000000000000004  7.9999999999999982   F   F   F
  1.9274052755876161  1.3575316072750010  9.2861208469999976   F   F   F
  3.1675737503083350  0.0000000000000005  9.2861208469999976   F   F   F
  3.1675737503083350  1.3575316072750012 12.5708101129999950   F   F   F
  3.1675737503083350  0.0000000000000006 11.2846892659999956   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416939999988   F   F   F
  4.4077422250290548  1.3575316072750010  9.2861208469999976   F   F   F
  5.0949790258959506  1.3575316072750012 12.5708101129999950   F   F   F
  0.0000000000000007  0.0000000000000007 12.5708101129999950   F   F   F
 19.0056510844787532  1.3576259825169552 16.0128546485473322   T   T   T
  0.0001895866969435  0.0000019202913793 14.5908031333326864   T   T   T
  3.1675737503083350  0.0000000000000008 13.8569309599999944   F   F   F
  1.2401684747207198  1.3575316072750012 12.5708101129999950   F   F   F
  1.9371815304548219  1.3575429407189716 15.9311772484091687   T   T   T
  3.1774049762616730  0.0000096233513608 15.9090025242830375   T   T   T
  3.1319200956071329  1.3575207695606810 19.2868719920610694   T   T   T
  3.2840949267807251 -0.0000519838906633 17.9241367426985079   T   T   T
 19.0054941680856011  0.0000316922455158 17.2943175816259682   T   T   T
  4.4916555876102695  1.3575410242463883 15.8441994822832708   T   T   T
  5.0953092510129183  1.3575450294531484 19.6799382851391229   T   T   T
 -0.0000621917844261  0.0000196892263183 19.9292113416096477   T   T   T
  3.1091896291048897 -0.0000346562456965 20.6522344967555007   T   T   T
  1.2284672183366807  1.3575453197981544 19.4347589783133579   T   T   T
  6.3351475006166700  1.3575316072750010  9.2861208469999976   F   F   F
  6.3351475006166700  0.0000000000000004  7.9999999999999982   F   F   F
  8.2625527762042843  1.3575316072750010  9.2861208469999976   F   F   F
  9.5027212509250027  0.0000000000000005  9.2861208469999976   F   F   F
  9.5027212509250027  1.3575316072750012 12.5708101129999950   F   F   F
  9.5027212509250027  0.0000000000000006 11.2846892659999956   F   F   F
  6.3351475006166700  0.0000000000000006 10.5722416939999988   F   F   F
 10.7428897256457230  1.3575316072750010  9.2861208469999976   F   F   F
 11.4301265265126197  1.3575316072750012 12.5708101129999950   F   F   F
  6.3351475006166700  0.0000000000000007 12.5708101129999950   F   F   F
  6.3481148541034056  1.3575224603680327 15.9354148535658950   T   T   T
  6.4709637924666703 -0.0000028724293035 14.6185755684443563   T   T   T
```

9.5027212509250027	0.0000000000000008	13.8569309599999944	F	F	F
7.5753159753373884	1.3575316072750012	12.5708101129999950	F	F	F
8.2567904175736473	1.3575377065679330	16.1483252377147508	T	T	T
9.5028475622043551	0.0000066805804936	15.8394329741974254	T	T	T
9.5026729542003938	1.3575999952342366	19.4834762183574597	T	T	T
9.5028036685402952	0.0000404287021949	18.1772945074747625	T	T	T
6.3033598451661446	0.0000003577122697	17.3906070277859861	T	T	T
10.7489114464915101	1.3575405413851149	16.1481445459517090	T	T	T
11.4303516608555640	1.3575520012446767	19.6891094337758084	T	T	T
6.3215811456552586	0.0000211877510884	19.2376391578337866	T	T	T
9.5026508167534445	0.0000107602196944	21.0100365416626929	T	T	T
7.5750659835750582	1.3575494124325895	19.6890441420691751	T	T	T
12.6702950012333382	1.3575316072750010	9.2861208469999976	F	F	F
12.6702950012333382	0.0000000000000004	7.9999999999999982	F	F	F
14.5977002768209552	1.3575316072750010	9.2861208469999976	F	F	F
15.8378687515416718	0.0000000000000005	9.2861208469999976	F	F	F
15.8378687515416718	1.3575316072750012	12.5708101129999950	F	F	F
15.8378687515416718	0.0000000000000006	11.2846892659999956	F	F	F
12.6702950012333382	0.0000000000000006	10.5722416939999988	F	F	F
17.0780372262623921	1.3575316072750010	9.2861208469999976	F	F	F
17.7652740271292870	1.3575316072750012	12.5708101129999950	F	F	F
12.6702950012333382	0.0000000000000007	12.5708101129999950	F	F	F
12.6576872458353957	1.3575131616925804	15.9353912553845056	T	T	T
12.5347521315046180	-0.0000197466459282	14.6185408833138748	T	T	T
15.8378687515416718	0.0000000000000008	13.8569309599999944	F	F	F
13.9104634759540549	1.3575316072750012	12.5708101129999950	F	F	F
14.5140949454414958	1.3575280680629083	15.8442570201420985	T	T	T
15.8284066099188934	-0.0000120634681329	15.9091046904581290	T	T	T
15.8733891134735767	1.3575097732747516	19.2869552155974979	T	T	T
15.7214551133731781	-0.0000167393305165	17.9241498738172531	T	T	T
12.7021808234934923	-0.0000058363311208	17.3905355518107072	T	T	T
17.0686099766724482	1.3575237242418170	15.9309496118248202	T	T	T
17.7768379519688580	1.3575444854873160	19.4347684513490506	T	T	T
12.6837375788373556	0.0000110411273302	19.2375473069182341	T	T	T
15.8960703336417843	-0.0000104819180284	20.6522969244231831	T	T	T
13.9100480138909042	1.3575461316264399	19.6798826038237351	T	T	T
-0.0000688680941382	-0.0000028892907736	22.4990977987542387	T	T	T
1.3485167331520878	1.3575268070006508	24.4066775337056505	T	T	T
-0.0000509559641537	-0.0000009185134105	26.2840642430916560	T	T	T
2.7489146915323599	-0.0000045431561007	22.6049213002841718	T	T	T
4.0640905239382068	1.3575311509346415	24.5001605844797226	T	T	T
2.6828666002162529	-0.0000015996910398	26.3193430032736302	T	T	T
5.4635581662436170	0.0000005244057331	22.6579847279283584	T	T	T
6.7993851946348727	1.3575311901438625	24.5005298960166229	T	T	T
5.4180242212270029	0.0000008326659835	26.3571900026156207	T	T	T
8.1047168602625383	-0.0000008609213207	22.6258604315674141	T	T	T
9.5026609009824341	1.3575290080500670	24.5163808928493943	T	T	T
8.1409607117667253	-0.0000033189980857	26.3476689587732231	T	T	T
10.9006094927871100	-0.0000022923748972	22.6258848610743435	T	T	T
12.2058672091447704	1.3575298051359583	24.5006296860670503	T	T	T
10.8643333509437561	-0.0000052832001114	26.3477051782960920	T	T	T
13.5417689998350070	-0.0000034243247417	22.6580283789226264	T	T	T
14.9412352065522587	1.3575268577484734	24.5001867800463309	T	T	T
13.5873014315115448	-0.0000048056750479	26.3572181706471973	T	T	T
16.2564172327046315	-0.0000074539256697	22.6049625727309476	T	T	T
17.6568185137360167	1.3574934533510592	24.4066830057652737	T	T	T
16.3224583524289422	-0.0000047917701550	26.3193616695667956	T	T	T

Oxide reference: TiO2(110)/fcc(100)_7x1/Ir E_tot= -625.88248417 eV
D3-zero damping= -11.1092304 eV, D3-BJ damping= -16.0365824 eV
Ti O Ti O Ti O Ti O Ti O Ti O Ti O Ti O Ti O Ti O Ti O Ti O Ti O Ti O Ti O
1.0000000000000000

```
    19.0054425018500055    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7150632145500007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6832577396346586
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.3575316072750010  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  8.0000000000000000   F   F   F
  1.9274052755876161  1.3575316072750010  9.2861208469999994   F   F   F
  3.1675737503083350  0.0000000000000005  9.2861208469999994   F   F   F
  3.1675737503083350  1.3575316072750012 12.5708101129999967   F   F   F
  3.1675737503083350  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.4077422250290548  1.3575316072750010  9.2861208469999994   F   F   F
  5.0949790258959506  1.3575316072750012 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000007 12.5708101129999967   F   F   F
 19.0054301336218145  1.3575316072750012 15.9186289785770310   T   T   T
 -0.0000184675711043  0.0000000000000018 14.6579890936497605   T   T   T
  3.1675737503083350  0.0000000000000008 13.8569309599999961   F   F   F
  1.2401684747207198  1.3575316072750012 12.5708101129999967   F   F   F
  1.9005055967525264  1.3575316072750012 16.0583268233508711   T   T   T
  3.1675547817000140  0.0000000000000009 16.3707019968803671   T   T   T
  3.1675828760097637  1.3575316072750017 19.8058651121767220   T   T   T
  3.1674934339374712  0.0000000000000009 18.2394358306503257   T   T   T
 19.0054731798755085  0.0000000000000011 17.3917727185231890   T   T   T
  4.4346281454414482  1.3575316072750012 16.0583932230181219   T   T   T
  5.1248008828086080  1.3575316072750017 19.7248494048958314   T   T   T
  0.0000392160296526  0.0000000000000011 19.2200725344073007   T   T   T
  3.1676330799799874  0.0000000000000012 21.0158898608031599   T   T   T
  1.2103374371341569  1.3575316072750017 19.7250525401252261   T   T   T
  6.3351475006166700  1.3575316072750010  9.2861208469999994   F   F   F
  6.3351475006166700  0.0000000000000004  8.0000000000000000   F   F   F
  8.2625527762042843  1.3575316072750010  9.2861208469999994   F   F   F
  9.5027212509250027  0.0000000000000005  9.2861208469999994   F   F   F
  9.5027212509250027  1.3575316072750012 12.5708101129999967   F   F   F
  9.5027212509250027  0.0000000000000006 11.2846892659999973   F   F   F
  6.3351475006166700  0.0000000000000006 10.5722416940000006   F   F   F
 10.7428897256457230  1.3575316072750010  9.2861208469999994   F   F   F
 11.4301265265126197  1.3575316072750012 12.5708101129999967   F   F   F
  6.3351475006166700  0.0000000000000007 12.5708101129999967   F   F   F
  6.3351403426287662  1.3575316072750012 15.9186351492779430   T   T   T
  6.3351349262528664  0.0000000000000009 14.6579942706717326   T   T   T
  9.5027212509250027  0.0000000000000008 13.8569309599999961   F   F   F
  7.5753159753373884  1.3575316072750012 12.5708101129999967   F   F   F
  8.2356580930733223  1.3575316072750012 16.0583307008966898   T   T   T
  9.5027038984713741  0.0000000000000009 16.3707063544785818   T   T   T
  9.5027354300647477  1.3575316072750017 19.8058665598206183   T   T   T
  9.5026435150633226  0.0000000000000010 18.2394391562951981   T   T   T
  6.3351864803234923  0.0000000000000010 17.3917755031974934   T   T   T
 10.7697770718316015  1.3575316072750012 16.0583930786147953   T   T   T
 11.4599501818354721  1.3575316072750017 19.7248440646757004   T   T   T
  6.3351881104032914  0.0000000000000011 19.2200782839851669   T   T   T
  9.5027834541490090  0.0000000000000012 21.0158910968664365   T   T   T
  7.5454874334417319  1.3575316072750017 19.7250560345608186   T   T   T
 12.6702950012333382  1.3575316072750010  9.2861208469999994   F   F   F
 12.6702950012333382  0.0000000000000004  8.0000000000000000   F   F   F
 14.5977002768209552  1.3575316072750010  9.2861208469999994   F   F   F
 15.8378687515416718  0.0000000000000005  9.2861208469999994   F   F   F
 15.8378687515416718  1.3575316072750012 12.5708101129999967   F   F   F
 15.8378687515416718  0.0000000000000006 11.2846892659999973   F   F   F
 12.6702950012333382  0.0000000000000006 10.5722416940000006   F   F   F
 17.0780372262623921  1.3575316072750010  9.2861208469999994   F   F   F
```

```
 17.7652740271292870  1.3575316072750012 12.5708101129999967   F   F   F
 12.6702950012333382  0.0000000000000007 12.5708101129999967   F   F   F
 12.6702876968400773  1.3575316072750012 15.9186309415176002   T   T   T
 12.6702848518159357  0.0000000000000009 14.6579907099525304   T   T   T
 15.8378687515416718  0.0000000000000008 13.8569309599999961   F   F   F
 13.9104634759540549  1.3575316072750012 12.5708101129999967   F   F   F
 14.5708043090346582  1.3575316072750012 16.0583379843993477   T   T   T
 15.8378491507325805  0.0000000000000009 16.3707280785337801   T   T   T
 15.8378793027227527  1.3575316072750017 19.8058896504668738   T   T   T
 15.8377845600455327  0.0000000000000010 18.2394561155097392   T   T   T
 12.6703257384955705  0.0000000000000010 17.3917763984019516   T   T   T
 17.1049201325391742  1.3575316072750012 16.0584047135775272   T   T   T
 17.7950942449078937  1.3575316072750017 19.7248444566855277   T   T   T
 12.6703378261881312  0.0000000000000011 19.2200766621795012   T   T   T
 15.8379340309309562  0.0000000000000011 21.0159125448210098   T   T   T
 13.8806341119356951  1.3575316072750017 19.7250669251690454   T   T   T

Metal reference: TiO2(110)/fcc(100)_7x1/Ir E_tot= -176.17406869 eV
 D3-zero damping= -8.6798938 eV, D3-BJ damping= -9.4085779 eV
Ir
 1.0000000000000000
    19.0054425018500055    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7150632145500007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.1817301592405194
  21
Cartesian
 -0.0001790770006071 -0.0000000000000002  8.3607466033697992
  1.3571229053304630  1.3575316072750003 10.2156972797405832
 -0.0002464990508917  0.0000000000000000 12.0706302935786489
  2.7140011783071865 -0.0000000000000000  8.3607764009064347
  4.0716004000238115  1.3575316072750003 10.2150083675414791
  2.7147723731553954  0.0000000000000000 12.0696802990961096
  5.4291832546159169 -0.0000000000000000  8.3606044591616371
  6.7877570788333310  1.3575316072750003 10.2142028494896309
  5.4303267723741397  0.0000000000000000 12.0689212551411575
  8.1460768936608883  0.0000000000000000  8.3602978416159619
  9.5027356315574192  1.3575316072750003 10.2157479433832066
  8.1445694864221494 -0.0000000000000000 12.0693878674296968
 10.8593952818836232  0.0000000000000000  8.3602609704798336
 12.2176243145833077  1.3575316072750003 10.2142060889378925
 10.8608173048449856  0.0000000000000000 12.0693683075693645
 13.5759939046237985  0.0000000000000000  8.3602567077177969
 14.9334503195766590  1.3575316072750003 10.2144379956832214
 13.5749623604730214 -0.0000000000000000 12.0688567095503938
 16.2914345386869108 -0.0000000000000000  8.3606399151782007
 17.6479666933159756  1.3575316072750003 10.2158999273447648
 16.2898332785578752  0.0000000000000000 12.0695723785879920

Interface: TiO2(110)/fcc(100)_7x1/Rh E_tot= -769.97704438 eV
 D3-zero damping= -22.6167446 eV, D3-BJ damping= -28.2279717 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Rh
 1.0000000000000000
    18.7436388669600049    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.6776626952800004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.2561367997801653
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2  21
Selective dynamics
Cartesian
  0.0000000000000006  1.3388313476400009  9.2861208469999976   F   F   F
  0.0000000000000005  0.0000000000000004  7.9999999999999982   F   F   F
  1.9008548962946381  1.3388313476400009  9.2861208469999976   F   F   F
```

3.1239398111600014	0.0000000000000005	9.2861208469999976	F	F	F
3.1239398111600014	1.3388313476400011	12.5708101129999950	F	F	F
3.1239398111600014	0.0000000000000006	11.2846892659999956	F	F	F
0.0000000000000006	0.0000000000000006	10.5722416939999988	F	F	F
4.3470247260253654	1.3388313476400009	9.2861208469999976	F	F	F
5.0247947074546389	1.3388313476400011	12.5708101129999950	F	F	F
0.0000000000000007	0.0000000000000007	12.5708101129999950	F	F	F
18.7437572808008888	1.3387059430896908	16.0221671467846285	T	T	T
0.0006809293215772	-0.0000068228498091	14.5929033605285152	T	T	T
3.1239398111600014	0.0000000000000008	13.8569309599999944	F	F	F
1.2230849148653642	1.3388313476400011	12.5708101129999950	F	F	F
1.9251591736809006	1.3388218783471586	15.9472119615514121	T	T	T
3.1672129797584918	-0.0000129149568283	15.9638752912542312	T	T	T
3.1014964126929301	1.3388981871151773	19.3613640477974549	T	T	T
3.3047349784445164	-0.0000073050285643	17.9646019245139428	T	T	T
18.7433793434854010	-0.0000443723341306	17.3131688159174466	T	T	T
4.4698980887110711	1.3388212792645644	15.7727941637139430	T	T	T
5.0393071671697216	1.3387990720165277	19.8397656785360716	T	T	T
0.0001262902002705	-0.0000261980634220	20.0344611452456753	T	T	T
3.0614874653490425	-0.0000128101042293	20.7217216967426801	T	T	T
1.2076443705841908	1.3388042032134926	19.4659230657039224	T	T	T
6.2478796223200028	1.3388313476400009	9.2861208469999976	F	F	F
6.2478796223200028	0.0000000000000004	7.9999999999999982	F	F	F
8.1487345186146403	1.3388313476400009	9.2861208469999976	F	F	F
9.3718194334800025	0.0000000000000005	9.2861208469999976	F	F	F
9.3718194334800025	1.3388313476400011	12.5708101129999950	F	F	F
9.3718194334800025	0.0000000000000006	11.2846892659999956	F	F	F
6.2478796223200028	0.0000000000000006	10.5722416939999988	F	F	F
10.5949043483453682	1.3388313476400009	9.2861208469999976	F	F	F
11.2726743297746417	1.3388313476400011	12.5708101129999950	F	F	F
6.2478796223200028	0.0000000000000007	12.5708101129999950	F	F	F
6.3064643627863584	1.3387553796635510	15.9544703104908603	T	T	T
6.4917201391528225	-0.0000420948946793	14.6230850904546372	T	T	T
9.3718194334800025	0.0000000000000008	13.8569309599999944	F	F	F
7.4709645371853668	1.3388313476400011	12.5708101129999950	F	F	F
8.1739365364408538	1.3388030269768538	16.3038685924862214	T	T	T
9.3723390636821016	-0.0000317365495802	15.7968937832167615	T	T	T
9.3718326557294613	1.3387559640060060	19.6164821700222767	T	T	T
9.3718741367866372	-0.0000438720591071	18.3305714951973222	T	T	T
6.1869369702925869	-0.0000429331281295	17.4305599354457073	T	T	T
10.5703881816650167	1.3388033397588555	16.3043659379662600	T	T	T
11.2960814307571802	1.3388258687710004	19.8317824069573909	T	T	T
6.2336698005179318	-0.0000158362016546	19.2676055141218860	T	T	T
9.3713002844250024	-0.0000216430967011	21.1163402843797137	T	T	T
7.4475579522283759	1.3388009636838698	19.8313489140129882	T	T	T
12.4957592446400039	1.3388313476400009	9.2861208469999976	F	F	F
12.4957592446400039	0.0000000000000004	7.9999999999999982	F	F	F
14.3966141409346431	1.3388313476400009	9.2861208469999976	F	F	F
15.6196990558000053	0.0000000000000005	9.2861208469999976	F	F	F
15.6196990558000053	1.3388313476400011	12.5708101129999950	F	F	F
15.6196990558000053	0.0000000000000006	11.2846892659999956	F	F	F
12.4957592446400039	0.0000000000000006	10.5722416939999988	F	F	F
16.8427839706653693	1.3388313476400009	9.2861208469999976	F	F	F
17.5205539520946409	1.3388313476400011	12.5708101129999950	F	F	F
12.4957592446400039	0.0000000000000007	12.5708101129999950	F	F	F
12.4378954303906539	1.3388340472862876	15.9544328734904983	T	T	T
12.2519491766277362	-0.0000004400480244	14.6232069864049237	T	T	T
15.6196990558000053	0.0000000000000008	13.8569309599999944	F	F	F
13.7188441595053643	1.3388313476400011	12.5708101129999950	F	F	F
14.2741631986879405	1.3388319225080385	15.7726072012079523	T	T	T
15.5767919355383651	0.0000007430331458	15.9644632772121540	T	T	T
15.6423237556447727	1.3387069209152394	19.3610855730150604	T	T	T
15.4396710971729654	-0.0000483070548523	17.9639632034421091	T	T	T

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 12.5571792705534158  0.0000031112934310 17.4306319600483306   T   T   T
 16.8188541855153062  1.3388341936153150 15.9452649112226883   T   T   T
 17.5360512387737941  1.3388069917183787 19.4657172590278975   T   T   T
 12.5096847396517941 -0.0000029029837928 19.2675063759603802   T   T   T
 15.6817312574307373 -0.0000524500395512 20.7213041211549474   T   T   T
 13.7043611795243834  1.3388265513111177 19.8390606497145150   T   T   T
 -0.0000914557418540  0.0001426519266088 22.5252398982840134   T   T   T
  1.3170391615140975  1.3389511958977280 24.4556647994415250   T   T   T
 -0.0002104877334393  0.0002173945111043 26.3208746921299372   T   T   T
  2.6720512110620915  0.0001601070177309 22.6614087425881010   T   T   T
  4.0061090513405437  1.3390031712738484 24.5156669086026611   T   T   T
  2.6577025866488944  0.0000944603816699 26.3329847870762883   T   T   T
  5.3630298277575070  0.0001494064307041 22.6602188570169467   T   T   T
  6.6875287026832062  1.3389377605919655 24.5021593386947458   T   T   T
  5.3372077698113403  0.0001775962532821 26.3595398125346243   T   T   T
  7.9937695183246458  0.0000764064087646 22.6757303041519869   T   T   T
  9.3713869964024372  1.3389556292278630 24.5627991100757015   T   T   T
  8.0073782338450599  0.0000855794809699 26.3536969608874756   T   T   T
 10.7498471297504796 -0.0000172945578082 22.6757735833125160   T   T   T
 12.0560043494018494  1.3388271034290806 24.5017202553338436   T   T   T
 10.7364413220726558  0.0001052229535325 26.3531076831838860   T   T   T
 13.3814309823227280 -0.0000496886585736 22.6596821325330744   T   T   T
 14.7372306219803360  1.3387747373870993 24.5151382623904190   T   T   T
 13.4051894972627981 -0.0000499808398840 26.3590254145521925   T   T   T
 16.0712552659541004  0.0000559294065601 22.6613508806918205   T   T   T
 17.4259445314841699  1.3389316390949453 24.4557338541519442   T   T   T
 16.0845199489982171 -0.0000925170770304 26.3330846449455436   T   T   T

Oxide reference: TiO2(110)/fcc(100)_7x1/Rh E_tot= -619.60427125 eV
 D3-zero damping= -11.2446236 eV, D3-BJ damping= -16.2709522 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O
 1.0000000000000000
    18.7436388669600049    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.6776626952800004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6832577396346586
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.3388313476400009  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  8.0000000000000000   F   F   F
  1.9008548962946381  1.3388313476400009  9.2861208469999994   F   F   F
  3.1239398111600014  0.0000000000000005  9.2861208469999994   F   F   F
  3.1239398111600014  1.3388313476400011 12.5708101129999967   F   F   F
  3.1239398111600014  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.3470247260253654  1.3388313476400009  9.2861208469999994   F   F   F
  5.0247947074546389  1.3388313476400011 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000007 12.5708101129999967   F   F   F
 18.7435925610869099  1.3388309642529916 15.9615842603525078   T   T   T
 -0.0000591862706271 -0.0000002561721057 14.6892342144004449   T   T   T
  3.1239398111600014  0.0000000000000008 13.8569309599999961   F   F   F
  1.2230849148653642  1.3388313476400011 12.5708101129999967   F   F   F
  1.8850032406743176  1.3388313476400011 16.1632442412810526   T   T   T
  3.1238850810386309 -0.0000000068625522 16.6040651011795504   T   T   T
  3.1240435753537978  1.3388313580128415 20.0483936018199280   T   T   T
  3.1238351952826475  0.0000000000000009 18.4477020448210567   T   T   T
 18.7437195551603146 -0.0000002263208568 17.4728804684404970   T   T   T
  4.3628336727087609  1.3388313476400011 16.1634190650548675   T   T   T
  5.0517603664649622  1.3388313693012206 19.8686268869973972   T   T   T
  0.0001604499694168  0.0000000327261018 19.2976748275416270   T   T   T
  3.1240849616764104 -0.0000000103728401 21.2709829870877947   T   T   T
```

```
  1.1962448595153452  1.3388313519722739 19.8689695174313101   T   T   T
  6.2478796223200028  1.3388313476400009  9.2861208469999994   F   F   F
  6.2478796223200028  0.0000000000000004  8.0000000000000000   F   F   F
  8.1487345186146403  1.3388313476400009  9.2861208469999994   F   F   F
  9.3718194334800025  0.0000000000000005  9.2861208469999994   F   F   F
  9.3718194334800025  1.3388313476400011 12.5708101129999967   F   F   F
  9.3718194334800025  0.0000000000000006 11.2846892659999973   F   F   F
  6.2478796223200028  0.0000000000000006 10.5722416940000006   F   F   F
 10.5949043483453682  1.3388313476400009  9.2861208469999994   F   F   F
 11.2726743297746417  1.3388313476400011 12.5708101129999967   F   F   F
  6.2478796223200028  0.0000000000000007 12.5708101129999967   F   F   F
  6.2478320232288809  1.3388312371561653 15.9615839556639560   T   T   T
  6.2478199832636312 -0.0000000873472503 14.6892339716636187   T   T   T
  9.3718194334800025  0.0000000000000008 13.8569309599999961   F   F   F
  7.4709645371853668  1.3388313476400011 12.5708101129999967   F   F   F
  8.1328819581170020  1.3388313476400011 16.1632409322153912   T   T   T
  9.3717536052627786 -0.0000000229906981 16.6040995014250221   T   T   T
  9.3719223110027308  1.3388313372671616 20.0483883394991054   T   T   T
  9.3717147499163502  0.0000000000000010 18.4476980296475510   T   T   T
  6.2479597066542967 -0.0000000620690204 17.4728802906277494   T   T   T
 10.6107141538357173  1.3388313402454723 16.1634185066584806   T   T   T
 11.2996397054984357  1.3388313584035003 19.8686222097826999   T   T   T
  6.2480387423010662  0.0000000118423575 19.2976747858448867   T   T   T
  9.3719647406230564  0.0000000103728424 21.2709780356159648   T   T   T
  7.4441231302976574  1.3388313497900328 19.8689691889556883   T   T   T
 12.4957592446400039  1.3388313476400009  9.2861208469999994   F   F   F
 12.4957592446400039  0.0000000000000004  8.0000000000000000   F   F   F
 14.3966141409346431  1.3388313476400009  9.2861208469999994   F   F   F
 15.6196990558000053  0.0000000000000005  9.2861208469999994   F   F   F
 15.6196990558000053  1.3388313476400011 12.5708101129999967   F   F   F
 15.6196990558000053  0.0000000000000006 11.2846892659999973   F   F   F
 12.4957592446400039  0.0000000000000006 10.5722416940000006   F   F   F
 16.8427839706653693  1.3388313476400009  9.2861208469999994   F   F   F
 17.5205539520946409  1.3388313476400011 12.5708101129999967   F   F   F
 12.4957592446400039  0.0000000000000007 12.5708101129999967   F   F   F
 12.4957131564554356  1.3388316299058629 15.9615844736821693   T   T   T
 12.4957005723307226  0.0000001572267353 14.6892343686686733   T   T   T
 15.6196990558000053  0.0000000000000008 13.8569309599999961   F   F   F
 13.7188441595053643  1.3388313476400011 12.5708101129999967   F   F   F
 14.3807630486776645  1.3388313476400011 16.1632427703902444   T   T   T
 15.6196448014140419  0.0000000000000009 16.6040642613716010   T   T   T
 15.6198024216251241  1.3388313873397861 20.0483928092637385   T   T   T
 15.6195939692031249  0.0000000000000010 18.4477013843276616   T   T   T
 12.4958401042529665  0.0000000541716882 17.4728803574329561   T   T   T
 16.8585941347941670  1.3388313735248627 16.1634202856055822   T   T   T
 17.5475196097450947  1.3388313666225997 19.8686238194525409   T   T   T
 12.4959198000960594 -0.0000000024367728 19.2976748583223241   T   T   T
 15.6198451918713133  0.0000000000000011 21.2709822944515636   T   T   T
 13.6920033583369030  1.3388313573452149 19.8689719650148469   T   T   T

Metal reference: TiO2(110)/fcc(100)_7x1/Rh E_tot= -145.07157006 eV
 D3-zero damping= -7.0107853 eV, D3-BJ damping= -8.4553159 eV
Rh
 1.0000000000000000
    18.7436388669600049    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.6776626952800004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.1817301592405194
  21
Cartesian
 -0.0002434475851483 -0.0000000000000003  8.3839008684893273
  1.3384433223390408  1.3388313476400002 10.2284371416898274
 -0.0001377387188917 -0.0000000000000000 12.0710430783145508
  2.6704048158374878 -0.0000000000000000  8.3820470157113558
```

```
  4.0157257012050218  1.3388313476400002 10.2217713910371693
  2.6812961315374140  0.0000000000000000 12.0680129792500352
  5.3474950490814877  0.0000000000000000  8.3704905128388081
  6.6964775963422847  1.3388313476400002 10.2043875299479616
  5.3639485623008323  0.0000000000000000 12.0543640414072240
  8.0286200923360678  0.0000000000000000  8.3561665517281938
  9.3716935341491183  1.3388313476400002 10.1973292196878234
  8.0361756983154535 -0.0000000000000000 12.0458076960865146
 10.7146646582048177  0.0000000000000000  8.3562079957706867
 12.0470491284652947  1.3388313476400002 10.2041725721222321
 10.7073930123038803  0.0000000000000000 12.0457566172630486
 13.3957334547289229  0.0000000000000000  8.3704311140495058
 14.7275583672472923  1.3388313476400002 10.2216987740306404
 13.3795869600652360 -0.0000000000000000 12.0543854996154387
 16.0728993926957315 -0.0000000000000000  8.3820090229180000
 17.4050702243734605  1.3388313476400002 10.2286961078998058
 16.0622441792772932  0.0000000000000000 12.0680847442969217

Interface: TiO2(110)/fcc(100)_7x1/Os E_tot= -846.59793057 eV
 D3-zero damping= -20.8546114 eV, D3-BJ damping= -27.5111064 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Os
 1.0000000000000000
    18.9588999815600054    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7084142830800007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.2561367997801653
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2  21
Selective dynamics
Cartesian
  0.0000000000000006  1.3542071415400010  9.2861208469999976   F   F   F
  0.0000000000000005  0.0000000000000004  7.9999999999999982   F   F   F
  1.9226852434632729  1.3542071415400010  9.2861208469999976   F   F   F
  3.1598166635933347  0.0000000000000005  9.2861208469999976   F   F   F
  3.1598166635933347  1.3542071415400012 12.5708101129999950   F   F   F
  3.1598166635933347  0.0000000000000006 11.2846892659999956   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416939999988   F   F   F
  4.3969480837233972  1.3542071415400010  9.2861208469999976   F   F   F
  5.0825019070566073  1.3542071415400012 12.5708101129999950   F   F   F
  0.0000000000000007  0.0000000000000007 12.5708101129999950   F   F   F
 18.9588963164511668  1.3542068677659327 16.0141290665672926   T   T   T
  0.0000473707120180  0.0000106204997822 14.5882910095706304   T   T   T
  3.1598166635933347  0.0000000000000008 13.8569309599999944   F   F   F
  1.2371314201300629  1.3542071415400012 12.5708101129999950   F   F   F
  1.9413385309496620  1.3542061964570598 15.9600994984888569   T   T   T
  3.1849237348102784 -0.0000018074277530 15.8931643859443046   T   T   T
  3.1242830405389359  1.3542055233406298 19.2905536903842361   T   T   T
  3.3006155518804885 -0.0000002927861610 17.9437736893204800   T   T   T
 18.9588470521658614  0.0000402300567908 17.2925319657884629   T   T   T
  4.4996683512656075  1.3542055094993899 15.8479652269448774   T   T   T
  5.0743271064721913  1.3542199778849431 19.7572328830427679   T   T   T
  0.0000076256445202 -0.0000015800463593 19.9417622382362332   T   T   T
  3.0629712076628266  0.0000014640977830 20.6996883874567139   T   T   T
  1.2283074013711688  1.3542077385559912 19.4161843943253487   T   T   T
  6.3196333271866694  1.3542071415400010  9.2861208469999976   F   F   F
  6.3196333271866694  0.0000000000000004  7.9999999999999982   F   F   F
  8.2423185706499407  1.3542071415400010  9.2861208469999976   F   F   F
  9.4794499907800027  0.0000000000000005  9.2861208469999976   F   F   F
  9.4794499907800027  1.3542071415400012 12.5708101129999950   F   F   F
  9.4794499907800027  0.0000000000000006 11.2846892659999956   F   F   F
  6.3196333271866694  0.0000000000000006 10.5722416939999988   F   F   F
 10.7165814109100666  1.3542071415400010  9.2861208469999976   F   F   F
 11.4021352342432767  1.3542071415400012 12.5708101129999950   F   F   F
```

6.3196333271866694	0.0000000000000007	12.5708101129999950	F	F	F
6.3609853566716810	1.3542028765973029	15.9559265825176055	T	T	T
6.4960406200462604	-0.0000026022442842	14.6243269804639731	T	T	T
9.4794499907800027	0.0000000000000008	13.8569309599999944	F	F	F
7.5567647473167323	1.3542071415400012	12.5708101129999950	F	F	F
8.2576663349985608	1.3542047613810000	16.2328381856292907	T	T	T
9.4794119431467543	-0.0000023941471534	15.7937556413284703	T	T	T
9.4795001760475888	1.3542058905134420	19.5908776581621495	T	T	T
9.4795453457390035	-0.0000033362239426	18.3277898135703019	T	T	T
6.2828619661297873	-0.0000019291016042	17.4259784964034559	T	T	T
10.7011953229142946	1.3542052303903704	16.2327476356051292	T	T	T
11.4096391760433402	1.3542070480764583	19.7691332876710213	T	T	T
6.2974002559039333	0.0000054825448119	19.2662303816376657	T	T	T
9.4794082664346959	0.0000000424509636	21.1695117794363732	T	T	T
7.5493602941771352	1.3542201822193771	19.7689887663164470	T	T	T
12.6392666543733370	1.3542071415400010	9.2861208469999976	F	F	F
12.6392666543733370	0.0000000000000004	7.9999999999999982	F	F	F
14.5619518978366127	1.3542071415400010	9.2861208469999976	F	F	F
15.7990833179666712	0.0000000000000005	9.2861208469999976	F	F	F
15.7990833179666712	1.3542071415400012	12.5708101129999950	F	F	F
15.7990833179666712	0.0000000000000006	11.2846892659999956	F	F	F
12.6392666543733370	0.0000000000000006	10.5722416939999988	F	F	F
17.0362147380967350	1.3542071415400010	9.2861208469999976	F	F	F
17.7217685614299434	1.3542071415400012	12.5708101129999950	F	F	F
12.6392666543733370	0.0000000000000007	12.5708101129999950	F	F	F
12.5978747590439255	1.3542404068175278	15.9558801481774655	T	T	T
12.4628772498732214	0.0000152571365657	14.6242988897694772	T	T	T
15.7990833179666712	0.0000000000000008	13.8569309599999944	F	F	F
13.8763980745033972	1.3542071415400012	12.5708101129999950	F	F	F
14.4592022221006680	1.3542038081520007	15.8480495253639706	T	T	T
15.7739575574949953	-0.0000048647090214	15.8932034365257220	T	T	T
15.8346293921275354	1.3542163690899922	19.2905858368189591	T	T	T
15.6584010437713577	-0.0000032115071775	17.9437723865275309	T	T	T
12.6759594467235690	0.0000156284066667	17.4259320586989439	T	T	T
17.0175543639738187	1.3542040606653651	15.9599259102768016	T	T	T
17.7305890873022847	1.3542063439637135	19.4162569306471440	T	T	T
12.6615255095256902	-0.0000227474701631	19.2662342690174349	T	T	T
15.8959294417558361	-0.0000047461346965	20.6997141346679250	T	T	T
13.8846151149542845	1.3542062432999977	19.7571409297573659	T	T	T
-0.0000602858767378	-0.0000119339645539	22.5749556623718988	T	T	T
1.4015127912536649	1.3542057240980110	24.4184537580875727	T	T	T
-0.0000599990012378	0.0000029037082903	26.2912222343126558	T	T	T
2.7903144139363132	0.0000023660596218	22.6325106837871139	T	T	T
4.0390518328185001	1.3542107935409955	24.5403543626671663	T	T	T
2.6407626825890222	-0.0000012047996009	26.3637296969115127	T	T	T
5.5118078294777604	0.0000048453560550	22.7799074457768675	T	T	T
6.7963789262181287	1.3542137269036103	24.6292152105879047	T	T	T
5.3898714294215164	0.0000071913180520	26.4467061322529133	T	T	T
8.0440521920146324	0.0000034513011789	22.7037177694954302	T	T	T
9.4794053949287207	1.3542070185284021	24.5906203122140639	T	T	T
8.1262809461911409	0.0000025635165936	26.4512501501948911	T	T	T
10.9147687756913072	-0.0000099723987420	22.7037095715230279	T	T	T
12.1623765285405572	1.3541915628350436	24.6292148807132598	T	T	T
10.8324873185398420	-0.0000076016955108	26.4512652381705422	T	T	T
13.4470641644428195	0.0000064037087497	22.7799642951122223	T	T	T
14.9197483209530404	1.3541760400814742	24.5403954372109787	T	T	T
13.5688672994247899	-0.0000237276905857	26.4466943343714789	T	T	T
16.1684797517309100	-0.0000204677658285	22.6325584266812179	T	T	T
17.5573308599062514	1.3541867395073119	24.4184672128913931	T	T	T
16.3179789375723736	-0.0000329392765640	26.3637862680147954	T	T	T

Oxide reference: TiO2(110)/fcc(100)_7x1/Os E_tot= -624.86604546 eV
D3-zero damping= -11.1321592 eV, D3-BJ damping= -16.0745031 eV

```
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O
 1.0000000000000000
    18.9588999815600054    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7084142830800007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6832577396346586
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.3542071415400010  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  8.0000000000000000   F   F   F
  1.9226852434632729  1.3542071415400010  9.2861208469999994   F   F   F
  3.1598166635933347  0.0000000000000005  9.2861208469999994   F   F   F
  3.1598166635933347  1.3542071415400012 12.5708101129999967   F   F   F
  3.1598166635933347  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.3969480837233972  1.3542071415400010  9.2861208469999994   F   F   F
  5.0825019070566073  1.3542071415400012 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000007 12.5708101129999967   F   F   F
 18.9589091689305711  1.3542071415400012 15.9282021428166694   T   T   T
 -0.0000722364971713  0.0000000000000013 14.6656281054637940   T   T   T
  3.1598166635933347  0.0000000000000008 13.8569309599999961   F   F   F
  1.2371314201300629  1.3542071415400012 12.5708101129999967   F   F   F
  1.8975545461386265  1.3542071415400012 16.0793626219560224   T   T   T
  3.1598026370122647  0.0000000000000008 16.4141051542118674   T   T   T
  3.1598375856157084  1.3542071415400017 19.8497395000519923   T   T   T
  3.1596873707080917  0.0000000000000009 18.2779366624633930   T   T   T
 18.9589290294091093  0.0000000000000010 17.4093765848003912   T   T   T
  4.4220665079232724  1.3542071415400012 16.0794923013271500   T   T   T
  5.1119200859733249  1.3542071415400017 19.7537624475980671   T   T   T
  0.0000055022202594  0.0000000000000011 19.2371144915913312   T   T   T
  3.1598586741597168  0.0000000000000012 21.0618745298036849   T   T   T
  1.2076360213963342  1.3542071415400017 19.7541047464277284   T   T   T
  6.3196333271866694  1.3542071415400010  9.2861208469999994   F   F   F
  6.3196333271866694  0.0000000000000004  8.0000000000000000   F   F   F
  8.2423185706499407  1.3542071415400010  9.2861208469999994   F   F   F
  9.4794499907800027  0.0000000000000005  9.2861208469999994   F   F   F
  9.4794499907800027  1.3542071415400012 12.5708101129999967   F   F   F
  9.4794499907800027  0.0000000000000006 11.2846892659999973   F   F   F
  6.3196333271866694  0.0000000000000006 10.5722416940000006   F   F   F
 10.7165814109100666  1.3542071415400010  9.2861208469999994   F   F   F
 11.4021352342432767  1.3542071415400012 12.5708101129999967   F   F   F
  6.3196333271866694  0.0000000000000007 12.5708101129999967   F   F   F
  6.3196448362863196  1.3542071415400012 15.9281992787517019   T   T   T
  6.3195625223725616  0.0000000000000009 14.6656236503678254   T   T   T
  9.4794499907800027  0.0000000000000008 13.8569309599999961   F   F   F
  7.5567647473167323  1.3542071415400012 12.5708101129999967   F   F   F
  8.2171916903706439  1.3542071415400012 16.0793647969248994   T   T   T
  9.4794346312358790  0.0000000000000009 16.4141163728601214   T   T   T
  9.4794535455416842  1.3542071415400017 19.8497464417186542   T   T   T
  9.4793136956881394  0.0000000000000010 18.2779436799724380   T   T   T
  6.3196637891808507  0.0000000000000009 17.4093703036149599   T   T   T
 10.7416996229193362  1.3542071415400012 16.0794966551891534   T   T   T
 11.4315524359536198  1.3542071415400017 19.7537636949486419   T   T   T
  6.3196411668007739  0.0000000000000011 19.2371156067689029   T   T   T
  9.4794868586789427  0.0000000000000011 21.0618804699294841   T   T   T
  7.5272739659983623  1.3542071415400017 19.7541095238016737   T   T   T
 12.6392666543733370  1.3542071415400010  9.2861208469999994   F   F   F
 12.6392666543733370  0.0000000000000004  8.0000000000000000   F   F   F
 14.5619518978366127  1.3542071415400010  9.2861208469999994   F   F   F
 15.7990833179666712  0.0000000000000005  9.2861208469999994   F   F   F
 15.7990833179666712  1.3542071415400012 12.5708101129999967   F   F   F
```

```
 15.7990833179666712  0.0000000000000006 11.2846892659999973   F   F   F
 12.6392666543733370  0.0000000000000006 10.5722416940000006   F   F   F
 17.0362147380967350  1.3542071415400010  9.2861208469999994   F   F   F
 17.7217685614299434  1.3542071415400012 12.5708101129999967   F   F   F
 12.6392666543733370  0.0000000000000007 12.5708101129999967   F   F   F
 12.6392735645599981  1.3542071415400012 15.9282010288646365   T   T   T
 12.6391953432208233  0.0000000000000009 14.6656263424900803   T   T   T
 15.7990833179666712  0.0000000000000008 13.8569309599999961   F   F   F
 13.8763980745033972  1.3542071415400012 12.5708101129999967   F   F   F
 14.5368238470429034  1.3542071415400012 16.0793640865275833   T   T   T
 15.7990669945022439  0.0000000000000009 16.4141167061947755   T   T   T
 15.7991138190558793  1.3542071415400017 19.8497459227283777   T   T   T
 15.7989460689754555  0.0000000000000010 18.2779483424433415   T   T   T
 12.6392945528654153  0.0000000000000010 17.4093744742150527   T   T   T
 17.0613318380365868  1.3542071415400012 16.0794960564423626   T   T   T
 17.7511886612371974  1.3542071415400017 19.7537639312265121   T   T   T
 12.6392727252074017  0.0000000000000011 19.2371159812178831   T   T   T
 15.7991194094816745  0.0000000000000011 21.0618798996735457   T   T   T
 13.8469022501707979  1.3542071415400017 19.7541093813958177   T   T   T

Metal reference: TiO2(110)/fcc(100)_7x1/Os E_tot= -216.20037634 eV
 D3-zero damping= -6.7395377 eV, D3-BJ damping= -8.0802486 eV
Os
 1.0000000000000000
    18.9588999815600054    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7084142830800007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.1817301592405194
  21
Cartesian
 -0.0000934070660052 -0.0000000000000003  8.3695901118900125
  1.3536411476349364  1.3542071415400003 10.2244422736750522
 -0.0001119507510590 -0.0000000000000000 12.0785043792444302
  2.7044161021513453 -0.0000000000000000  8.3657408570919127
  4.0618189918918315  1.3542071415400003 10.2165639881151336
  2.7117706589112465  0.0000000000000000 12.0747546475063281
  5.4115058669135712 -0.0000000000000000  8.3585801886125406
  6.7705231599839975  1.3542071415400003 10.2073765247065182
  5.4204807452589856  0.0000000000000000 12.0669753229163508
  8.1238060561449537  0.0000000000000000  8.3540753170426747
  9.4793189846326964  1.3542071415400003 10.2061932536100066
  8.1252337401656387 -0.0000000000000000 12.0622238106571533
 10.8347446512082595  0.0000000000000000  8.3539466440933232
 12.1880662205459913  1.3542071415400003 10.2072607499988788
 10.8334825785681161  0.0000000000000000 12.0621403865745034
 13.5472046481195392  0.0000000000000000  8.3584100535784760
 14.8968318097795382  1.3542071415400003 10.2165203027438327
 13.5380249463022508 -0.0000000000000000 12.0668103957382584
 16.2544571924976502 -0.0000000000000000  8.3657659942070790
 17.6050313868053117  1.3542071415400003 10.2245323575338674
 16.2468965714057276  0.0000000000000000 12.0747926667611818

Interface: TiO2(110)/fcc(100)_9x1/Au E_tot= -945.98057084 eV
 D3-zero damping= -30.4008239 eV, D3-BJ damping= -34.98111 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Au
 1.0000000000000000
    26.0887653942300055    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8987517104700005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.4127819096326846
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2  27
Selective dynamics
```

Cartesian

0.0000000000000007	1.4493758552350009	9.2861208469999994	F	F	F
0.0000000000000005	0.0000000000000005	8.0000000000000000	F	F	F
1.9843114958851349	1.4493758552350009	9.2861208469999994	F	F	F
3.2610956742787516	0.0000000000000006	9.2861208469999994	F	F	F
3.2610956742787516	1.4493758552350011	12.5708101129999967	F	F	F
3.2610956742787516	0.0000000000000007	11.2846892659999973	F	F	F
0.0000000000000006	0.0000000000000006	10.5722416940000006	F	F	F
4.5378798526723685	1.4493758552350009	9.2861208469999994	F	F	F
5.2454071701638858	1.4493758552350011	12.5708101129999967	F	F	F
0.0000000000000008	0.0000000000000008	12.5708101129999967	F	F	F
26.0888359079934062	1.4493749553710575	15.8544037170500740	T	T	T
0.0000458585036878	-0.0000008369026878	14.6225708911129129	T	T	T
3.2610956742787516	0.0000000000000008	13.8569309599999961	F	F	F
1.2767841783936171	1.4493758552350011	12.5708101129999967	F	F	F
1.9635149815293942	1.4493719025588072	15.8969064096007173	T	T	T
3.2614577672923750	-0.0000094410898120	15.9419048808067370	T	T	T
3.2592510455214265	1.4494471886597819	19.2862898878068485	T	T	T
3.2721208572564460	0.0000297984752457	17.8962173133912827	T	T	T
26.0887218063092305	-0.0000004659103655	17.2540060071823014	T	T	T
4.5625421470136622	1.4493721041638574	15.8894631512917250	T	T	T
5.2860804142696720	1.4493839587460784	19.4082197465576947	T	T	T
-0.0000435389321062	0.0000041544499282	19.1072494678064437	T	T	T
3.2726920457892827	0.0000517265834747	20.4920361886137563	T	T	T
1.2517155219713352	1.4493843434934559	19.4042465775047930	T	T	T
6.5221913485575032	1.4493758552350009	9.2861208469999994	F	F	F
6.5221913485575032	0.0000000000000005	8.0000000000000000	F	F	F
8.5065028444426360	1.4493758552350009	9.2861208469999994	F	F	F
9.7832870228362516	0.0000000000000006	9.2861208469999994	F	F	F
9.7832870228362516	1.4493758552350011	12.5708101129999967	F	F	F
9.7832870228362516	0.0000000000000007	11.2846892659999973	F	F	F
6.5221913485575032	0.0000000000000006	10.5722416940000006	F	F	F
11.0600712012298690	1.4493758552350009	9.2861208469999994	F	F	F
11.7675985187213872	1.4493758552350011	12.5708101129999967	F	F	F
6.5221913485575032	0.0000000000000008	12.5708101129999967	F	F	F
6.5194356260345536	1.4493507853644125	15.8527567679078238	T	T	T
6.5312985235569156	-0.0000147892970416	14.6221589005379364	T	T	T
9.7832870228362516	0.0000000000000008	13.8569309599999961	F	F	F
7.7989755269511187	1.4493758552350011	12.5708101129999967	F	F	F
8.4878718432199616	1.4493693825663747	15.9088606280697427	T	T	T
9.7826995339186258	-0.0000087450857726	15.9442525781065392	T	T	T
9.7853327396797223	1.4494183057516636	19.3012965399195053	T	T	T
9.7849543170060453	0.0000053640658301	17.9233812187464530	T	T	T
6.5217657156286579	-0.0000119190061312	17.2538167366288242	T	T	T
11.0808402819579133	1.4493694354464286	15.9002700131632384	T	T	T
11.7938964511494415	1.4493774353456597	19.3645262437465959	T	T	T
6.5269323336488450	-0.0000016618258769	19.1029571502039204	T	T	T
9.8218577079160774	0.0000211660405869	20.5543087517197129	T	T	T
7.7884374367807609	1.4493779575707195	19.4050728399342667	T	T	T
13.0443826971150028	1.4493758552350009	9.2861208469999994	F	F	F
13.0443826971150028	0.0000000000000005	8.0000000000000000	F	F	F
15.0286941930001365	1.4493758552350009	9.2861208469999994	F	F	F
16.3054783713937539	0.0000000000000006	9.2861208469999994	F	F	F
16.3054783713937539	1.4493758552350011	12.5708101129999967	F	F	F
16.3054783713937539	0.0000000000000007	11.2846892659999973	F	F	F
13.0443826971150028	0.0000000000000006	10.5722416940000006	F	F	F
17.5822625497873659	1.4493758552350009	9.2861208469999994	F	F	F
18.2897898672788877	1.4493758552350011	12.5708101129999967	F	F	F
13.0443826971150028	0.0000000000000008	12.5708101129999967	F	F	F
13.0443444074168813	1.4493635246829377	15.8385760092316232	T	T	T
13.0444045514988094	-0.0000092376958896	14.6107515765023361	T	T	T
16.3054783713937539	0.0000000000000008	13.8569309599999961	F	F	F
14.3211668755086183	1.4493758552350011	12.5708101129999967	F	F	F

15.0078759727933733	1.4493572577979461	15.9002598966026003	T	T	T
16.3059416138456008	-0.0000354250431729	15.9442485136843448	T	T	T
16.3033630154105857	1.4493771595407472	19.3013972762352104	T	T	T
16.3037651455747152	-0.0000114524854924	17.9234253325119255	T	T	T
13.0444764399140585	-0.0000083790636194	17.2285836490478417	T	T	T
17.6008279089795145	1.4493581363123669	15.9089486511759439	T	T	T
18.3003318610619452	1.4493627460483631	19.4048354809749206	T	T	T
13.0443823008745259	-0.0000007299248072	19.0742109095449202	T	T	T
16.2670735269420454	-0.0000052104882933	20.5544084456278995	T	T	T
14.2948367022551128	1.4493745906473450	19.3647335756688079	T	T	T
19.5665740456725032	1.4493758552350009	9.2861208469999994	F	F	F
19.5665740456725032	0.0000000000000005	8.0000000000000000	F	F	F
21.5508855415576406	1.4493758552350009	9.2861208469999994	F	F	F
22.8276697199512526	0.0000000000000006	9.2861208469999994	F	F	F
22.8276697199512526	1.4493758552350011	12.5708101129999967	F	F	F
22.8276697199512526	0.0000000000000007	11.2846892659999973	F	F	F
19.5665740456725032	0.0000000000000006	10.5722416940000006	F	F	F
24.1044538983448717	1.4493758552350009	9.2861208469999994	F	F	F
24.8119812158363864	1.4493758552350011	12.5708101129999967	F	F	F
19.5665740456725032	0.0000000000000008	12.5708101129999967	F	F	F
19.5692317368137232	1.4493691852219759	15.8526850870504639	T	T	T
19.5574373239639243	-0.0000061523838659	14.6220365419225349	T	T	T
22.8276697199512526	0.0000000000000008	13.8569309599999961	F	F	F
20.8433582240661224	1.4493758552350011	12.5708101129999967	F	F	F
21.5262896441558951	1.4493750916515258	15.8895306769091480	T	T	T
22.8273701969363785	0.0000025121543775	15.9416186889006237	T	T	T
22.8295299088925816	1.4493820643867479	19.2861515194830986	T	T	T
22.8166493521339042	0.0000001126281524	17.8962383260202529	T	T	T
19.5670939379412197	-0.0000094194419679	17.2536070805633734	T	T	T
24.1253131601350113	1.4493763494975140	15.8969021284310159	T	T	T
24.8370088722351454	1.4493801488140829	19.4042668134589711	T	T	T
19.5618693596092257	0.0000120891311301	19.1028011692563382	T	T	T
22.8159220876007325	0.0000019362039582	20.4920657287102443	T	T	T
20.8025863185348605	1.4493643775627640	19.4081574836979662	T	T	T
-0.0000580419768051	-0.0000193529298056	22.4841158550041982	T	T	T
1.4141569477305067	1.4493573437521974	24.7311565476843498	T	T	T
-0.0001160491686768	0.0000485270495263	26.8063625161634640	T	T	T
2.7346765930651857	-0.0000017765769027	22.6601965255605649	T	T	T
4.2541664327851914	1.4493189131269069	24.6590842726723345	T	T	T
2.9014742804197140	-0.0000275847017686	26.8344735931794709	T	T	T
5.5509419547783700	0.0000338742132339	22.4660015013709646	T	T	T
7.1371766882879939	1.4493851169137404	24.5055716495863827	T	T	T
5.7851368910896452	-0.0000014269601984	26.6305480230472469	T	T	T
8.2707834099115072	0.0000051325391745	22.3176961636294102	T	T	T
10.0250386367911641	1.4493864845240079	24.1339918627141437	T	T	T
8.7274503176231697	0.0000226025420128	26.4235260144001352	T	T	T
11.6612274018165891	0.0000151854217039	22.2311362405053679	T	T	T
13.0440564890060458	1.4493901349805174	24.2948867101933708	T	T	T
11.5121677300135268	-0.0000536880343076	26.2333884649002549	T	T	T
14.4275503026749909	0.0000347754157201	22.2315656013155376	T	T	T
16.0642767615505910	1.4494006615628150	24.1338182397055014	T	T	T
14.5763801298978546	-0.0000489403980357	26.2328472506887067	T	T	T
17.8182693578931541	-0.0000005779693239	22.3175613434773261	T	T	T
18.9517913989039855	1.4493452870196437	24.5059064544023109	T	T	T
17.3610735032065833	-0.0000127764350350	26.4234435127764193	T	T	T
20.5379767376491458	-0.0000147492678776	22.4662329585287814	T	T	T
21.8348768182998860	1.4494055171164268	24.6592725340559049	T	T	T
20.3040959255798761	0.0000015755123180	26.6305153317497201	T	T	T
23.3540864548480336	0.0000308174336565	22.6602149185992907	T	T	T
24.6746736372661495	1.4493558986335433	24.7309020370212735	T	T	T
23.1877356955942950	-0.0000022722051653	26.8346822185917375	T	T	T

Oxide reference: TiO2(110)/fcc(100)_9x1/Au E_tot= -850.71016248 eV

```
 D3-zero damping= -13.8479071 eV, D3-BJ damping= -19.86784 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
    26.0887653942300055    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8987517104700005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.8017123208283969
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2
Selective dynamics
Cartesian
  0.0000000000000007  1.4493758552350009  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.9843114958851349  1.4493758552350009  9.2861208469999994   F   F   F
  3.2610956742787516  0.0000000000000006  9.2861208469999994   F   F   F
  3.2610956742787516  1.4493758552350011 12.5708101129999967   F   F   F
  3.2610956742787516  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.5378798526723685  1.4493758552350009  9.2861208469999994   F   F   F
  5.2454071701638858  1.4493758552350011 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000008 12.5708101129999967   F   F   F
 26.0887933946699206  1.4493758552350011 15.8297464066508144   T   T   T
  0.0000215247844945  0.0000000000000003 14.6154143524716815   T   T   T
  3.2610956742787516  0.0000000000000008 13.8569309599999961   F   F   F
  1.2767841783936171  1.4493758552350011 12.5708101129999967   F   F   F
  1.9597969050606865  1.4493758552350011 15.9104088915072381   T   T   T
  3.2612065596601165  0.0000000000000009 16.0446159484532167   T   T   T
  3.2611632390422574  1.4493758552350018 19.4300399622803894   T   T   T
  3.2615814219913872  0.0000000000000011 17.9313703670237210   T   T   T
 26.0887728785153357  0.0000000000000011 17.2218706190222228   T   T   T
  4.5625037739577099  1.4493758552350011 15.9100691080037588   T   T   T
  5.2902356274800866  1.4493758552350018 19.4120488829044469   T   T   T
  0.0000060039295701  0.0000000000000012 19.0583921985021227   T   T   T
  3.2608420796522295  0.0000000000000012 20.5634067778308598   T   T   T
  1.2320456565620437  1.4493758552350018 19.4113567714886024   T   T   T
  6.5221913485575032  1.4493758552350009  9.2861208469999994   F   F   F
  6.5221913485575032  0.0000000000000005  8.0000000000000000   F   F   F
  8.5065028444426360  1.4493758552350009  9.2861208469999994   F   F   F
  9.7832870228362516  0.0000000000000006  9.2861208469999994   F   F   F
  9.7832870228362516  1.4493758552350011 12.5708101129999967   F   F   F
  9.7832870228362516  0.0000000000000007 11.2846892659999973   F   F   F
  6.5221913485575032  0.0000000000000006 10.5722416940000006   F   F   F
 11.0600712012298690  1.4493758552350009  9.2861208469999994   F   F   F
 11.7675985187213872  1.4493758552350011 12.5708101129999967   F   F   F
  6.5221913485575032  0.0000000000000008 12.5708101129999967   F   F   F
  6.5222123209281353  1.4493758552350011 15.8298581198388302   T   T   T
  6.5221923444100387  0.0000000000000010 14.6155093786953856   T   T   T
  9.7832870228362516  0.0000000000000008 13.8569309599999961   F   F   F
  7.7989755269511187  1.4493758552350011 12.5708101129999967   F   F   F
  8.4818921728460452  1.4493758552350011 15.9100510011142635   T   T   T
  9.7832166961443683  0.0000000000000010 16.0445557201315800   T   T   T
  9.7832220247605584  1.4493758552350018 19.4300025387866029   T   T   T
  9.7828105673151775  0.0000000000000011 17.9313179388703965   T   T   T
  6.5221961108501070  0.0000000000000010 17.2221531061539963   T   T   T
 11.0846110986771134  1.4493758552350011 15.9103640794428625   T   T   T
 11.8123436961591324  1.4493758552350018 19.4113128809663174   T   T   T
  6.5221921086870909  0.0000000000000011 19.0587362258837558   T   T   T
  9.7835535862386163  0.0000000000000012 20.5633411549059559   T   T   T
  7.7541476422958873  1.4493758552350018 19.4120411286175560   T   T   T
 13.0443826971150028  1.4493758552350009  9.2861208469999994   F   F   F
 13.0443826971150028  0.0000000000000005  8.0000000000000000   F   F   F
 15.0286941930001365  1.4493758552350009  9.2861208469999994   F   F   F
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 16.3054783713937539  0.0000000000000006  9.2861208469999994   F   F   F
 16.3054783713937539  1.4493758552350011 12.5708101129999967   F   F   F
 16.3054783713937539  0.0000000000000007 11.2846892659999973   F   F   F
 13.0443826971150028  0.0000000000000006 10.5722416940000006   F   F   F
 17.5822625497873659  1.4493758552350009  9.2861208469999994   F   F   F
 18.2897898672788877  1.4493758552350011 12.5708101129999967   F   F   F
 13.0443826971150028  0.0000000000000008 12.5708101129999967   F   F   F
 13.0444108758501418  1.4493758552350011 15.8297463530534444   T   T   T
 13.0444045434230826  0.0000000000000009 14.6154143098685765   T   T   T
 16.3054783713937539  0.0000000000000008 13.8569309599999961   F   F   F
 14.3211668755086183  1.4493758552350011 12.5708101129999967   F   F   F
 15.0041797417023393  1.4493758552350011 15.9104091159709977   T   T   T
 16.3055893390580309  0.0000000000000009 16.0446164274274707   T   T   T
 16.3055460034311892  1.4493758552350018 19.4300405013638482   T   T   T
 16.3059642493447967  0.0000000000000011 17.9313707821796378   T   T   T
 13.0443903379092614  0.0000000000000011 17.2218705471551452   T   T   T
 17.6068864531379177  1.4493758552350011 15.9100693504424910   T   T   T
 18.3346182872214243  1.4493758552350018 19.4120492631290382   T   T   T
 13.0443889743497028  0.0000000000000011 19.0583921062980295   T   T   T
 16.3052248579368460  0.0000000000000012 20.5634072749407970   T   T   T
 14.2764285917691875  1.4493758552350018 19.4113568723278433   T   T   T
 19.5665740456725032  1.4493758552350009  9.2861208469999994   F   F   F
 19.5665740456725032  0.0000000000000005  8.0000000000000000   F   F   F
 21.5508855415576406  1.4493758552350009  9.2861208469999994   F   F   F
 22.8276697199512526  0.0000000000000006  9.2861208469999994   F   F   F
 22.8276697199512526  1.4493758552350011 12.5708101129999967   F   F   F
 22.8276697199512526  0.0000000000000007 11.2846892659999973   F   F   F
 19.5665740456725032  0.0000000000000006 10.5722416940000006   F   F   F
 24.1044538983448717  1.4493758552350009  9.2861208469999994   F   F   F
 24.8119812158363864  1.4493758552350011 12.5708101129999967   F   F   F
 19.5665740456725032  0.0000000000000008 12.5708101129999967   F   F   F
 19.5665949872796112  1.4493758552350011 15.8298582410302959   T   T   T
 19.5665749616524991  0.0000000000000009 14.6155095109834168   T   T   T
 22.8276697199512526  0.0000000000000008 13.8569309599999961   F   F   F
 20.8433582240661224  1.4493758552350011 12.5708101129999967   F   F   F
 21.5262748034849274  1.4493758552350011 15.9100512116832302   T   T   T
 22.8275992558256959  0.0000000000000009 16.0445563496203718   T   T   T
 22.8276044329545726  1.4493758552350018 19.4300032686275337   T   T   T
 22.8271929196484535  0.0000000000000011 17.9313184854418814   T   T   T
 19.5665787028497249  0.0000000000000010 17.2221533301873251   T   T   T
 24.1289936014135193  1.4493758552350011 15.9103645076288451   T   T   T
 24.8567260854644161  1.4493758552350018 19.4113131336946267   T   T   T
 19.5665746849264401  0.0000000000000011 19.0587364181877277   T   T   T
 22.8279360175238679  0.0000000000000012 20.5633418742262180   T   T   T
 20.7985301516605894  1.4493758552350018 19.4120415246059324   T   T   T

Metal reference: TiO2(110)/fcc(100)_9x1/Au E_tot= -90.04706624 eV
 D3-zero damping= -11.08433 eV, D3-BJ damping= -11.1938598 eV
Au
 1.0000000000000000
    26.0887653942300055    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8987517104700005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.0765597851474737
  27
Cartesian
  0.0002264889624438 -0.0000003508845090  7.9580136880792045
  1.4470673843432693  1.4493770494403928 10.0335591731435656
  0.0001802675157405 -0.0000001923329627 12.1090443834503514
  2.9007451971017022 -0.0000003795432594  7.9640466586173941
  4.3497344844229504  1.4493753427949956 10.0427002870183717
  2.8977026086364250  0.0000068344760067 12.1094679241744156
  5.8018085576513290 -0.0000008902795856  7.9730986627304263
  7.2587889971107860  1.4493812991896176 10.0405389611387594
```

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  5.8079824379090832 -0.0000022253368232 12.1111301494443211
  8.7060938748552346 -0.0000911705606203  7.9667944508420119
 10.1564594328098199  1.4493333291656152 10.0378586565528209
  8.7104120299897758 -0.0000249208626584 12.1151199509331171
 11.6001761194071698 -0.0000108203346251  7.9552206065368347
 13.0444385428122249  1.4493756459717042 10.0374948580187251
 11.6010093576669178 -0.0000102951258141 12.1184937030204019
 14.4884316166691605  0.0000082444202987  7.9555618586449146
 15.9322617107789082  1.4493761782309564 10.0379392082452803
 14.4877642018532384  0.0000980051895095 12.1187995030313793
 17.3823991605292107 -0.0000004202962268  7.9667478839071473
 18.8294580991505001  1.4493789149193335 10.0399777643137611
 17.3782638178968725  0.0000001092650864 12.1150912125037085
 20.2865525128655193  0.0000080847908030  7.9733947026889034
 21.7388909022664976  1.4493849332577602 10.0419969945314751
 20.2809072560289216  0.0000080569429551 12.1101657135958245
 23.1887159386836288  0.0000080463327167  7.9638946880666506
 24.6416420764662760  1.4493791185982470 10.0334873168032832
 23.1916015906501087  0.0000080450326487 12.1088939350064564

Interface: TiO2(110)/fcc(100)_9x1/Ag E_tot= -929.63536128 eV
 D3-zero damping= -27.3106555 eV, D3-BJ damping= -34.0363434 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ag
 1.0000000000000000
    25.9247434675500052    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8805270519500006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.4127819096326846
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2  27
Selective dynamics
Cartesian
  0.0000000000000007  1.4402635259750010  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.9718359881418541  1.4402635259750010  9.2861208469999994   F   F   F
  3.2405929334437515  0.0000000000000006  9.2861208469999994   F   F   F
  3.2405929334437515  1.4402635259750012 12.5708101129999967   F   F   F
  3.2405929334437515  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.5093498787456490  1.4402635259750010  9.2861208469999994   F   F   F
  5.2124289215856043  1.4402635259750012 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 25.9247213467473117  1.4402789790602593 15.8603868999314308   T   T   T
 -0.0000220635711033 -0.0000728000298336 14.6227823625678912   T   T   T
  3.2405929334437515  0.0000000000000008 13.8569309599999961   F   F   F
  1.2687569453018979  1.4402635259750012 12.5708101129999967   F   F   F
  1.9490293650446564  1.4402819770550108 15.9214528608453474   T   T   T
  3.2406704519427412  0.0000178609687287 15.9601208413014835   T   T   T
  3.2446288387893603  1.4402528986302348 19.3382714372021098   T   T   T
  3.2493595057012015  0.0000052855510681 17.9435533829040708   T   T   T
 25.9247135247358464  0.0000254765773682 17.2778048011601619   T   T   T
  4.5334186058927886  1.4402772229822072 15.9132689594591508   T   T   T
  5.2631942448709372  1.4402738634826673 19.4704741417715219   T   T   T
 -0.0000269146782787  0.0000112234544230 19.1163659066385385   T   T   T
  3.2880558911450506 -0.0000019034612975 20.5632711166659945   T   T   T
  1.2452925075028660  1.4402678181793898 19.4931466625060814   T   T   T
  6.4811858668875031  1.4402635259750010  9.2861208469999994   F   F   F
  6.4811858668875031  0.0000000000000005  8.0000000000000000   F   F   F
  8.4530218550293537  1.4402635259750010  9.2861208469999994   F   F   F
  9.7217788003312506  0.0000000000000006  9.2861208469999994   F   F   F
  9.7217788003312506  1.4402635259750012 12.5708101129999967   F   F   F
  9.7217788003312506  0.0000000000000007 11.2846892659999973   F   F   F
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6.4811858668875031	0.0000000000000006	10.5722416940000006	F	F	F
10.9905357456331494	1.4402635259750010	9.2861208469999994	F	F	F
11.6936147884731056	1.4402635259750012	12.5708101129999967	F	F	F
6.4811858668875031	0.0000000000000007	12.5708101129999967	F	F	F
6.4791241469790304	1.4402764781859336	15.8490262987751560	T	T	T
6.4824985000601947	0.0000065041814996	14.6124415038816640	T	T	T
9.7217788003312506	0.0000000000000008	13.8569309599999961	F	F	F
7.7499428121893992	1.4402635259750012	12.5708101129999967	F	F	F
8.4306111087551816	1.4402688211319696	15.9093275709177497	T	T	T
9.7214803291619329	0.0000056583486786	15.9227095502606950	T	T	T
9.7280068140897900	1.4402737364070923	19.2949893208901671	T	T	T
9.7271062670819735	0.0000006298220687	17.9273971700438324	T	T	T
6.4856827468645770	0.0000074580630365	17.2589260404904437	T	T	T
11.0142115456802028	1.4402675688306525	15.8998431839325107	T	T	T
11.7238557049115570	1.4402534395792663	19.4163056229987561	T	T	T
6.4953527702510998	0.0000146669800428	19.0954729677389778	T	T	T
9.7790776835340036	0.0000034184258994	20.5622634304227390	T	T	T
7.7481048597830746	1.4402745841936488	19.4612775729571439	T	T	T
12.9623717337750026	1.4402635259750010	9.2861208469999994	F	F	F
12.9623717337750026	0.0000000000000005	8.0000000000000000	F	F	F
14.9342077219168559	1.4402635259750010	9.2861208469999994	F	F	F
16.2029646672187511	0.0000000000000006	9.2861208469999994	F	F	F
16.2029646672187511	1.4402635259750012	12.5708101129999967	F	F	F
16.2029646672187511	0.0000000000000007	11.2846892659999973	F	F	F
12.9623717337750026	0.0000000000000006	10.5722416940000006	F	F	F
17.4717216125206463	1.4402635259750010	9.2861208469999994	F	F	F
18.1748006553606061	1.4402635259750012	12.5708101129999967	F	F	F
12.9623717337750026	0.0000000000000007	12.5708101129999967	F	F	F
12.9623517049167809	1.4402543774774956	15.8281450068887146	T	T	T
12.9623621044878963	-0.0000007820443644	14.5956729630763125	T	T	T
16.2029646672187511	0.0000000000000008	13.8569309599999961	F	F	F
14.2311286790768996	1.4402635259750012	12.5708101129999967	F	F	F
14.9105009816037235	1.4403205063898430	15.8998457235032991	T	T	T
16.2032250717328346	0.0000664665737151	15.9226902032900934	T	T	T
16.1967034316883698	1.4402267392485324	19.2949726016239111	T	T	T
16.1975973740849035	0.0000039468511367	17.9273774318779147	T	T	T
12.9623595776883835	-0.0000008501623598	17.2250493178956461	T	T	T
17.4940979893497186	1.4403151134022347	15.9093416257765039	T	T	T
18.1766022667255633	1.4402549854248692	19.4612500332696605	T	T	T
12.9623544430193682	-0.0000133457607950	19.0569275499931479	T	T	T
16.1456746503827979	-0.0000147420535714	20.5622418441304617	T	T	T
14.2008495637717775	1.4402518689081740	19.4163241495814276	T	T	T
19.4435576006625013	1.4402635259750010	9.2861208469999994	F	F	F
19.4435576006625013	0.0000000000000005	8.0000000000000000	F	F	F
21.4153935888043563	1.4402635259750010	9.2861208469999994	F	F	F
22.6841505341062550	0.0000000000000006	9.2861208469999994	F	F	F
22.6841505341062550	1.4402635259750012	12.5708101129999967	F	F	F
22.6841505341062550	0.0000000000000007	11.2846892659999973	F	F	F
19.4435576006625013	0.0000000000000006	10.5722416940000006	F	F	F
23.9529074794081538	1.4402635259750010	9.2861208469999994	F	F	F
24.6559865222481065	1.4402635259750012	12.5708101129999967	F	F	F
19.4435576006625013	0.0000000000000007	12.5708101129999967	F	F	F
19.4455658559214299	1.4402569274120318	15.8490696264666440	T	T	T
19.4422315607801011	0.0000017623690802	14.6124603772387225	T	T	T
22.6841505341062550	0.0000000000000008	13.8569309599999961	F	F	F
20.7123145459644036	1.4402635259750012	12.5708101129999967	F	F	F
21.3912936865529382	1.4402694385386046	15.9132930339121330	T	T	T
22.6840255062171465	0.0000040030530190	15.9601355859402627	T	T	T
22.6800760856417583	1.4402603273398753	19.3382280144233789	T	T	T
22.6753437641743822	0.0000003403930172	17.9435694985418586	T	T	T
19.4390408894853266	0.0000030099080811	17.2589908835943433	T	T	T
23.9756757724012424	1.4402754731479510	15.9214521157433904	T	T	T
24.6793956682431848	1.4402673175863729	19.4931525622648145	T	T	T

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 19.4293774216751807 -0.0000097236030317 19.0955724111886198   T   T   T
 22.6366436099352448 -0.0000021896760501 20.5632892480799647   T   T   T
 20.6615345005508608  1.4402559827763837 19.4705096980747108   T   T   T
  0.0001003835968359  0.0000032033010360 22.6544976414273123   T   T   T
  1.4254504503369072  1.4402699111762745 24.7722634084493052   T   T   T
  0.0000578693913645  0.0000055754893742 26.8194860420992853   T   T   T
  2.7272438565802291  0.0000030296986137 22.6876625810850676   T   T   T
  4.2621326209283961  1.4402632866879292 24.6260544213114159   T   T   T
  2.9369660756826867  0.0000034994649950 26.7926467882182102   T   T   T
  5.5384424826167979 -0.0000019639254757 22.4065658715096454   T   T   T
  7.1046911367370846  1.4402615757466208 24.3954338825373966   T   T   T
  5.8104921333367381 -0.0000018369054861 26.5661435218110427   T   T   T
  8.3064561298369579  0.0000278726112303 22.2874663061702236   T   T   T
 10.0064246515517326  1.4402611817017408 24.1847141450124603   T   T   T
  8.6958912151172552 -0.0000025498514215 26.3465636752888130   T   T   T
 11.5364438746685867 -0.0000127936240114 22.1674893897521237   T   T   T
 12.9624239036747930  1.4402344058828975 24.1602567443371896   T   T   T
 11.5135603617799980 -0.0000062970745986 26.2113475500979689   T   T   T
 14.3883599783527423 -0.0000306181344378 22.1674764128380311   T   T   T
 15.9184458544660732  1.4402579076345683 24.1846506255787972   T   T   T
 14.4112537652551822 -0.0000320400860695 26.2113669092187145   T   T   T
 17.6183581135987097  0.0000356394199029 22.2874749036057267   T   T   T
 18.8202083637987911  1.4402468136322111 24.3953403727746689   T   T   T
 17.2289635503489045 -0.0000103531294765 26.3464615517039142   T   T   T
 20.3864606821269447  0.0000249455226220 22.4065337564732268   T   T   T
 21.6627154866281977  1.4402730517940407 24.6260130233220771   T   T   T
 20.1143544870347526 -0.0000023736453546 26.5660671173130574   T   T   T
 23.1977291053794090  0.0000060377499021 22.6876479914923017   T   T   T
 24.4994218721641630  1.4402676037159527 24.7723238216190076   T   T   T
 22.9878119451308827  0.0000064517247996 26.7926401323946983   T   T   T

Oxide reference: TiO2(110)/fcc(100)_9x1/Ag E_tot= -849.85201961 eV
 D3-zero damping= -13.9824752 eV, D3-BJ damping= -20.0945939 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
    25.9247434675500052    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8805270519500006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.8017123208283969
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2
Selective dynamics
Cartesian
  0.0000000000000007  1.4402635259750010  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.9718359881418541  1.4402635259750010  9.2861208469999994   F   F   F
  3.2405929334437515  0.0000000000000006  9.2861208469999994   F   F   F
  3.2405929334437515  1.4402635259750012 12.5708101129999967   F   F   F
  3.2405929334437515  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.5093498787456490  1.4402635259750010  9.2861208469999994   F   F   F
  5.2124289215856043  1.4402635259750012 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 25.9247697230578709  1.4403031231419816 15.8323469612568886   T   T   T
 -0.0002109505152670  0.0000365816604856 14.6145545331689082   T   T   T
  3.2405929334437515  0.0000000000000008 13.8569309599999961   F   F   F
  1.2687569453018979  1.4402635259750012 12.5708101129999967   F   F   F
  1.9466732341242754  1.4403436284430189 15.9188233355506821   T   T   T
  3.2406510637010570  0.0000192096669518 16.0653837432774438   T   T   T
  3.2405732391700082  1.4402907620913556 19.4579945221246895   T   T   T
  3.2405892345848200  0.0000355646349097 17.9515043845560918   T   T   T
 25.9248813633877226 -0.0000006105709397 17.2316727786880151   T   T   T
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4.5346167406822140	1.4402442614398294	15.9189639338607964	T	T	T
5.2544884135647880	1.4402115549916452	19.4347311217764656	T	T	T
-0.0001060245260438	0.0000056535134338	19.0662511853922645	T	T	T
3.2403010258406417	0.0000238769974550	20.5992311869552829	T	T	T
1.2265508490799708	1.4403050398252675	19.4340526713169268	T	T	T
6.4811858668875031	1.4402635259750010	9.2861208469999994	F	F	F
6.4811858668875031	0.0000000000000005	8.0000000000000000	F	F	F
8.4530218550293537	1.4402635259750010	9.2861208469999994	F	F	F
9.7217788003312506	0.0000000000000006	9.2861208469999994	F	F	F
9.7217788003312506	1.4402635259750012	12.5708101129999967	F	F	F
9.7217788003312506	0.0000000000000007	11.2846892659999973	F	F	F
6.4811858668875031	0.0000000000000006	10.5722416940000006	F	F	F
10.9905357456331494	1.4402635259750010	9.2861208469999994	F	F	F
11.6936147884731056	1.4402635259750012	12.5708101129999967	F	F	F
6.4811858668875031	0.0000000000000007	12.5708101129999967	F	F	F
6.4811885493063723	1.4403154683936681	15.8326255217049603	T	T	T
6.4813435316770960	0.0000403063738522	14.6147575441853519	T	T	T
9.7217788003312506	0.0000000000000008	13.8569309599999961	F	F	F
7.7499428121893992	1.4402635259750012	12.5708101129999967	F	F	F
8.4278045881716626	1.4403555504443766	15.9193334235954094	T	T	T
9.7218295004409150	-0.0000525358613806	16.0656291464994503	T	T	T
9.7219490207307633	1.4402350167307620	19.4579643715019159	T	T	T
9.7218593843141328	0.0000162589429230	17.9516773828566620	T	T	T
6.4810988973088719	-0.0000018737758320	17.2321387557739918	T	T	T
11.0157909026084528	1.4402317961650104	15.9192800342478797	T	T	T
11.7358153118916242	1.4402165233647137	19.4342691025949641	T	T	T
6.4812494922699457	0.0000042309679327	19.0667271822095969	T	T	T
9.7221982873616017	-0.0000246495025203	20.5990999622573234	T	T	T
7.7079295651114084	1.4402940962843449	19.4349219904926045	T	T	T
12.9623717337750026	1.4402635259750010	9.2861208469999994	F	F	F
12.9623717337750026	0.0000000000000005	8.0000000000000000	F	F	F
14.9342077219168559	1.4402635259750010	9.2861208469999994	F	F	F
16.2029646672187511	0.0000000000000006	9.2861208469999994	F	F	F
16.2029646672187511	1.4402635259750012	12.5708101129999967	F	F	F
16.2029646672187511	0.0000000000000007	11.2846892659999973	F	F	F
12.9623717337750026	0.0000000000000006	10.5722416940000006	F	F	F
17.4717216125206463	1.4402635259750010	9.2861208469999994	F	F	F
18.1748006553606061	1.4402635259750012	12.5708101129999967	F	F	F
12.9623717337750026	0.0000000000000007	12.5708101129999967	F	F	F
12.9624718652283732	1.4402057426470125	15.8325312780704035	T	T	T
12.9624540676584665	-0.0000238248597348	14.6147020231991736	T	T	T
16.2029646672187511	0.0000000000000008	13.8569309599999961	F	F	F
14.2311286790768996	1.4402635259750012	12.5708101129999967	F	F	F
14.9090365695485225	1.4402331883748598	15.9193721404954935	T	T	T
16.2029955302131725	-0.0000345196580009	16.0657276057144784	T	T	T
16.2028499937614612	1.4401763384528463	19.4582255396284722	T	T	T
16.2028751107895985	0.0000216180451254	17.9518464821626154	T	T	T
12.9625183101109567	-0.0000244763605704	17.2318079191196141	T	T	T
17.4969072629472144	1.4402157623747402	15.9193736205311183	T	T	T
18.2169154244631351	1.4401565862280084	19.4348863137971861	T	T	T
12.9624764397430194	0.0000028426900293	19.0663209459573082	T	T	T
16.2026424554275117	-0.0001017421060054	20.5994210985274542	T	T	T
14.1890388252967057	1.4402839064805835	19.4344554907142566	T	T	T
19.4435576006625013	1.4402635259750010	9.2861208469999994	F	F	F
19.4435576006625013	0.0000000000000005	8.0000000000000000	F	F	F
21.4153935888043563	1.4402635259750010	9.2861208469999994	F	F	F
22.6841505341062550	0.0000000000000006	9.2861208469999994	F	F	F
22.6841505341062550	1.4402635259750012	12.5708101129999967	F	F	F
22.6841505341062550	0.0000000000000007	11.2846892659999973	F	F	F
19.4435576006625013	0.0000000000000006	10.5722416940000006	F	F	F
23.9529074794081538	1.4402635259750010	9.2861208469999994	F	F	F
24.6559865222481065	1.4402635259750012	12.5708101129999967	F	F	F
19.4435576006625013	0.0000000000000007	12.5708101129999967	F	F	F

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 19.4435782815634965  1.4402462610268625 15.8326944573085910   T   T   T
 19.4435889798647246 -0.0000327097273767 14.6148507211777350   T   T   T
 22.6841505341062550  0.0000000000000008 13.8569309599999961   F   F   F
 20.7123145459644036  1.4402635259750012 12.5708101129999967   F   F   F
 21.3902378839012073  1.4401685512964042 15.9192607132263539   T   T   T
 22.6841781016311685 -0.0001598414152668 16.0662766987370809   T   T   T
 22.6841139922554689  1.4402564846738433 19.4579775942889874   T   T   T
 22.6842248037306291 -0.0000321171781960 17.9520113274958923   T   T   T
 19.4433688276121437 -0.0000398145657369 17.2321752316146366   T   T   T
 23.9780365122940928  1.4402616595287754 15.9190523960170989   T   T   T
 24.6979868278415324  1.4402768115029190 19.4344449598717866   T   T   T
 19.4435135982407310 -0.0000684312881312 19.0667843353281157   T   T   T
 22.6843788106594459 -0.0000183392824797 20.5989057688676738   T   T   T
 20.6702262563750025  1.4401369554656451 19.4350173766757912   T   T   T

Metal reference: TiO2(110)/fcc(100)_9x1/Ag E_tot= -73.68445506 eV
 D3-zero damping= -8.0854471 eV, D3-BJ damping= -10.1783455 eV
Ag
 1.0000000000000000
    25.9247434675500052    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8805270519500006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.0765597851474737
  27
Cartesian
  0.0000041450151184  0.0000001697089990  7.9825513409694917
  1.4391401874600842  1.4402636914649933 10.0467082657496025
  0.0001119519941144 -0.0000001110745513 12.1122257109584108
  2.8790621768558959 -0.0000002427743833  7.9799265068801768
  4.3213585512470063  1.4402638889125887 10.0409859808325983
  2.8808414883136328  0.0000003564283042 12.1083046617328129
  5.7579259251520654  0.0000004009402233  7.9725107301473974
  7.2047980081149348  1.4402633710170689 10.0304623205305035
  5.7620869443544604  0.0000000575796910 12.0997410645467056
  8.6450438462949233 -0.0000011494533388  7.9686876747353645
 10.0822533162477441  1.4402628615766944 10.0345702017397773
  8.6397779245146307 -0.0000003862858122 12.0996425760784234
 11.5251693859087023 -0.0000004938604273  7.9715319586087432
 12.9624026072935177  1.4402631168212945 10.0381909749478986
 11.5203754010630046 -0.0000000715438545 12.0993847394392642
 14.3994941101623528 -0.0000001643259138  7.9716420822942622
 15.8424009841901388  1.4402638109775985 10.0345394234976073
 14.4044390023374245 -0.0000000575796910 12.0992557473011981
 17.2795759504807265 -0.0000002892216051  7.9686096882914947
 18.7198786886623871  1.4402637508807576 10.0304726940192257
 17.2850611778356722  0.0000001707637560 12.0994563731309093
 20.1667527416935819  0.0000008721361673  7.9726267459979594
 21.6034106455715893  1.4402640231320902 10.0412834655873962
 20.1626721263259938  0.0000004988535664 12.0998151281959991
 23.0456830613638779 -0.0000001668803878  7.9800607225479725
 24.4856064332983792  1.4402637061228538 10.0467813813906144
 23.0441191193134642  0.0000006035995767 12.1085676196878378

Interface: TiO2(110)/fcc(100)_9x1/Pt E_tot= -1004.16950361 eV
 D3-zero damping= -32.7799874 eV, D3-BJ damping= -38.9595204 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Pt
 1.0000000000000000
    24.9340802887800024    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7704533654200003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.4127819096326846
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2  27
```

```
Selective dynamics
Cartesian
  0.0000000000000006  1.3852266827100008  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.8964861467646077  1.3852266827100008  9.2861208469999994   F   F   F
  3.1167600360975012  0.0000000000000005  9.2861208469999994   F   F   F
  3.1167600360975012  1.3852266827100010 12.5708101129999967   F   F   F
  3.1167600360975012  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.3370339254303945  1.3852266827100008  9.2861208469999994   F   F   F
  5.0132461828621082  1.3852266827100010 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000007 12.5708101129999967   F   F   F
 24.9341126160344011  1.3852265738510412 15.8915035083449467   T   T   T
 -0.0000098924053152 -0.0000000689209027 14.6020076062666107   T   T   T
  3.1167600360975012  0.0000000000000008 13.8569309599999961   F   F   F
  1.2202738893328939  1.3852266827100010 12.5708101129999967   F   F   F
  1.8673252264344697  1.3852267685022375 15.9124126328048128   T   T   T
  3.1180092893343336  0.0000000864558877 15.9777464191614929   T   T   T
  3.1134999828892620  1.3852269949907778 19.3588760906017079   T   T   T
  3.0836021248809287  0.0000002159033714 17.9529872551949161   T   T   T
 24.9341372214646704  0.0000000000000010 17.3294515477634938   T   T   T
  4.3759150256520796  1.3852267510543588 15.9739088310605233   T   T   T
  5.0338067916267821  1.3852270296205389 19.5373256463780471   T   T   T
  0.0000337670101856  0.0000003854610220 19.1824021213219069   T   T   T
  3.1284359935498709  0.0000002827039976 20.6665380252988875   T   T   T
  1.2046171826517154  1.3852269980506082 19.6115065487525015   T   T   T
  6.2335200721950024  1.3852266827100008  9.2861208469999994   F   F   F
  6.2335200721950024  0.0000000000000005  8.0000000000000000   F   F   F
  8.1300062189596076  1.3852266827100008  9.2861208469999994   F   F   F
  9.3502801082925018  0.0000000000000005  9.2861208469999994   F   F   F
  9.3502801082925018  1.3852266827100010 12.5708101129999967   F   F   F
  9.3502801082925018  0.0000000000000006 11.2846892659999973   F   F   F
  6.2335200721950024  0.0000000000000006 10.5722416940000006   F   F   F
 10.5705539976253942  1.3852266827100008  9.2861208469999994   F   F   F
 11.2467662550571088  1.3852266827100010 12.5708101129999967   F   F   F
  6.2335200721950024  0.0000000000000007 12.5708101129999967   F   F   F
  6.2398961284879659  1.3852271099225875 15.8934389952175916   T   T   T
  6.2214619906139168  0.0000002618396732 14.6075004924870822   T   T   T
  9.3502801082925018  0.0000000000000008 13.8569309599999961   F   F   F
  7.4537939615278948  1.3852266827100010 12.5708101129999967   F   F   F
  8.1082041062211978  1.3852266660539325 15.9017271734089558   T   T   T
  9.3470007645743731 -0.0000000056569202 16.0566982827866447   T   T   T
  9.3383054928001172  1.3852268083486594 19.4565800791807533   T   T   T
  9.2893116660260446  0.0000002296527448 18.0340542341046657   T   T   T
  6.2845302020369784  0.0000001782644543 17.3423445748950371   T   T   T
 10.6003112301425642  1.3852266903723145 15.9789944695184847   T   T   T
 11.2491702484513088  1.3852278882128735 19.5346045350733633   T   T   T
  6.2608371430778602  0.0000003770452280 19.1893897175206263   T   T   T
  9.4400213792404557  0.0000003215207082 20.8501685196307314   T   T   T
  7.4442004455981765  1.3852270317384971 19.7242634150442591   T   T   T
 12.4670401443900012  1.3852266827100008  9.2861208469999994   F   F   F
 12.4670401443900012  0.0000000000000005  8.0000000000000000   F   F   F
 14.3635262911546082  1.3852266827100008  9.2861208469999994   F   F   F
 15.5838001804875024  0.0000000000000005  9.2861208469999994   F   F   F
 15.5838001804875024  1.3852266827100010 12.5708101129999967   F   F   F
 15.5838001804875024  0.0000000000000006 11.2846892659999973   F   F   F
 12.4670401443900012  0.0000000000000006 10.5722416940000006   F   F   F
 16.8040740698203948  1.3852266827100008  9.2861208469999994   F   F   F
 17.4802863272521094  1.3852266827100010 12.5708101129999967   F   F   F
 12.4670401443900012  0.0000000000000007 12.5708101129999967   F   F   F
 12.4670689615231005  1.3852289493797421 15.8728996523997932   T   T   T
 12.4671241271116671  0.0000013084095116 14.5977381577289957   T   T   T
 15.5838001804875024  0.0000000000000008 13.8569309599999961   F   F   F
```

13.6873140337228953	1.3852266827100010	12.5708101129999967	F	F	F
14.3338285961596288	1.3852264746998739	15.9790582060341055	T	T	T
15.5871630206852725	-0.0000002520924465	16.0565510271911336	T	T	T
15.5957523073740632	1.3852266276534391	19.4565405248930432	T	T	T
15.6447851822600743	0.0000001387913137	18.0340178609725719	T	T	T
12.4670862191932308	0.0000010279675671	17.3101169519370295	T	T	T
16.8259374810919127	1.3852264330913033	15.9017887588303761	T	T	T
17.4898741590838682	1.3852273658255976	19.7242518447949742	T	T	T
12.4670226275705076	0.0000014498423596	19.1455716599247552	T	T	T
15.4940131956206706	0.0000002483142557	20.8502179228623099	T	T	T
13.6848820586852398	1.3852279185161509	19.5346589959531833	T	T	T
18.7005602165850036	1.3852266827100008	9.2861208469999994	F	F	F
18.7005602165850036	0.0000000000000005	8.0000000000000000	F	F	F
20.5970463633496124	1.3852266827100008	9.2861208469999994	F	F	F
21.8173202526825030	0.0000000000000005	9.2861208469999994	F	F	F
21.8173202526825030	1.3852266827100010	12.5708101129999967	F	F	F
21.8173202526825030	0.0000000000000006	11.2846892659999973	F	F	F
18.7005602165850036	0.0000000000000006	10.5722416940000006	F	F	F
23.0375941420153971	1.3852266827100008	9.2861208469999994	F	F	F
23.7138063994471082	1.3852266827100010	12.5708101129999967	F	F	F
18.7005602165850036	0.0000000000000007	12.5708101129999967	F	F	F
18.6942333678577235	1.3852301729508882	15.8934364151394334	T	T	T
18.7126186217948671	0.0000017672734005	14.6075113880528544	T	T	T
21.8173202526825030	0.0000000000000008	13.8569309599999961	F	F	F
19.9208341059178977	1.3852266827100010	12.5708101129999967	F	F	F
20.5582164851998108	1.3852266106585076	15.9738809464062257	T	T	T
21.8161088681013453	-0.0000000893577762	15.9778014854846049	T	T	T
21.8204552495754243	1.3852270367173791	19.3589657342448191	T	T	T
21.8504222447860990	0.0000002200706872	17.9530926629504428	T	T	T
18.6496303468926143	0.0000013118862743	17.3423262613008795	T	T	T
23.0667852361650247	1.3852266541296741	15.9124958993705246	T	T	T
23.7295145684125615	1.3852270233569244	19.6114156132116371	T	T	T
18.6731930004584363	0.0000008155115768	19.1894361964081099	T	T	T
21.8056958487471775	0.0000003358167320	20.6666365089272936	T	T	T
19.9002514849913617	1.3852273820638707	19.5373826668093891	T	T	T
0.0001132426753319	-0.0000000150419609	22.6529564635249550	T	T	T
1.3934725937010588	1.3852266766232944	24.6263706355791747	T	T	T
0.0002130283917303	-0.0000001068300554	26.5715300942507717	T	T	T
2.6951154988696784	-0.0000000682444313	22.6387085664369820	T	T	T
4.1524838200247967	1.3852267895400563	24.6101540357646513	T	T	T
2.7898779257409307	0.0000002387599026	26.5571552064648877	T	T	T
5.4766277858414822	-0.0000000327875348	22.6203704380686013	T	T	T
6.9188111407414539	1.3852265336734821	24.5556295330227137	T	T	T
5.5831546957522962	-0.0000001098734095	26.5310689541064804	T	T	T
8.1326653098565824	-0.0000003694600215	22.5460736835624722	T	T	T
9.6949602272251845	1.3852265543999491	24.4028492280082894	T	T	T
8.3706754993709005	-0.0000001952514434	26.4286676511236962	T	T	T
11.1238847056247288	-0.0000001088589581	22.4218450428521194	T	T	T
12.4671216395908502	1.3852267945077308	24.3821204950282713	T	T	T
11.0967360420699084	0.0000002369727606	26.3387318028470077	T	T	T
13.8101898582978855	0.0000001629010703	22.4218391377095578	T	T	T
15.2393661592683340	1.3852267915689600	24.4027620622766506	T	T	T
13.8376541718071753	0.0000001098734095	26.3386337108713597	T	T	T
16.8016083734274062	-0.0000001129167636	22.5460536709893908	T	T	T
18.0153553911301536	1.3852267472622926	24.5555160095123632	T	T	T
16.5634852403520085	-0.0000000010144514	26.4286983869256247	T	T	T
19.4576692599960595	0.0000001687480609	22.6201272497965107	T	T	T
20.7817381961053655	1.3852269014423670	24.6101170941148482	T	T	T
19.3509149891892278	0.0000001588432648	26.5310995354273373	T	T	T
22.2390072743707492	0.0000001700022298	22.6388659762910791	T	T	T
23.5407379063400768	1.3852268085311394	24.6264573252402812	T	T	T
22.1444031594426249	0.0000002595866120	26.5569902934768187	T	T	T

```
Oxide reference: TiO2(110)/fcc(100)_9x1/Pt E_tot= -836.69910618 eV
 D3-zero damping= -14.7277043 eV, D3-BJ damping= -21.3214287 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
    24.9340802887800024    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7704533654200003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.8017123208283969
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.3852266827100008  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.8964861467646077  1.3852266827100008  9.2861208469999994   F   F   F
  3.1167600360975012  0.0000000000000005  9.2861208469999994   F   F   F
  3.1167600360975012  1.3852266827100010 12.5708101129999967   F   F   F
  3.1167600360975012  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.3370339254303945  1.3852266827100008  9.2861208469999994   F   F   F
  5.0132461828621082  1.3852266827100010 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000007 12.5708101129999967   F   F   F
 24.9340217259659838  1.3852266827100010 15.8827434861684527   T   T   T
 -0.0000323913536531  0.0000000000000009 14.6480956480434603   T   T   T
  3.1167600360975012  0.0000000000000008 13.8569309599999961   F   F   F
  1.2202738893328939  1.3852266827100010 12.5708101129999967   F   F   F
  1.8783221503329675  1.3852266827100010 16.0566103756304948   T   T   T
  3.1162744807127698  0.0000000000000008 16.3782881447399618   T   T   T
  3.1154730335243959  1.3852266827100015 19.8129202073338249   T   T   T
  3.1108186601278147  0.0000000000000010 18.2371495598377820   T   T   T
 24.9340060051521881  0.0000000000000011 17.3543422378683232   T   T   T
  4.3552185613468319  1.3852266827100010 16.0596211826190753   T   T   T
  5.0472289235171006  1.3852266827100015 19.6778312043022083   T   T   T
 -0.0000761884827985  0.0000000000000011 19.1733154481594887   T   T   T
  3.1175123566164626  0.0000000000000011 20.9973289790317210   T   T   T
  1.1839105829915129  1.3852266827100015 19.6859100684569093   T   T   T
  6.2335200721950024  1.3852266827100008  9.2861208469999994   F   F   F
  6.2335200721950024  0.0000000000000005  8.0000000000000000   F   F   F
  8.1300062189596076  1.3852266827100008  9.2861208469999994   F   F   F
  9.3502801082925018  0.0000000000000005  9.2861208469999994   F   F   F
  9.3502801082925018  1.3852266827100010 12.5708101129999967   F   F   F
  9.3502801082925018  0.0000000000000006 11.2846892659999973   F   F   F
  6.2335200721950024  0.0000000000000006 10.5722416940000006   F   F   F
 10.5705539976253942  1.3852266827100008  9.2861208469999994   F   F   F
 11.2467662550571088  1.3852266827100010 12.5708101129999967   F   F   F
  6.2335200721950024  0.0000000000000007 12.5708101129999967   F   F   F
  6.2334801604272192  1.3852266827100010 15.8817088112900429   T   T   T
  6.2334536088404855  0.0000000000000010 14.6472875075050410   T   T   T
  9.3502801082925018  0.0000000000000008 13.8569309599999961   F   F   F
  7.4537939615278948  1.3852266827100010 12.5708101129999967   F   F   F
  8.1117654130009598  1.3852266827100010 16.0595922548934453   T   T   T
  9.3506792003900472  0.0000000000000009 16.3783141840530782   T   T   T
  9.3513493801686174  1.3852266827100015 19.8128823393954114   T   T   T
  9.3559875021122885  0.0000000000000011 18.2371496769101888   T   T   T
  6.2334472286444171  0.0000000000000010 17.3529591524788032   T   T   T
 10.5886022649552611  1.3852266827100010 16.0566472006279994   T   T   T
 11.2829027826364179  1.3852266827100015 19.6858586220540488   T   T   T
  6.2334202845444944  0.0000000000000011 19.1709191017321885   T   T   T
  9.3491997843186301  0.0000000000000012 20.9972740890643443   T   T   T
  7.4195565442447728  1.3852266827100015 19.6777780424156852   T   T   T
 12.4670401443900012  1.3852266827100008  9.2861208469999994   F   F   F
 12.4670401443900012  0.0000000000000005  8.0000000000000000   F   F   F
```

```
 14.3635262911546082  1.3852266827100008  9.2861208469999994   F   F   F
 15.5838001804875024  0.0000000000000005  9.2861208469999994   F   F   F
 15.5838001804875024  1.3852266827100010 12.5708101129999967   F   F   F
 15.5838001804875024  0.0000000000000006 11.2846892659999973   F   F   F
 12.4670401443900012  0.0000000000000006 10.5722416940000006   F   F   F
 16.8040740698203948  1.3852266827100008  9.2861208469999994   F   F   F
 17.4802863272521094  1.3852266827100010 12.5708101129999967   F   F   F
 12.4670401443900012  0.0000000000000007 12.5708101129999967   F   F   F
 12.4669670898658467  1.3852266827100010 15.8827419236858880   T   T   T
 12.4669940002051227  0.0000000000000009 14.6480924252536795   T   T   T
 15.5838001804875024  0.0000000000000008 13.8569309599999961   F   F   F
 13.6873140337228953  1.3852266827100010 12.5708101129999967   F   F   F
 14.3453485400142444  1.3852266827100010 16.0566127272405410   T   T   T
 15.5833015061827727  0.0000000000000009 16.3782936197507496   T   T   T
 15.5825048891387432  1.3852266827100015 19.8129262506155612   T   T   T
 15.5778525799688961  0.0000000000000010 18.2371549898696301   T   T   T
 12.4669591856919357  0.0000000000000010 17.3543464338136140   T   T   T
 16.8222450602883811  1.3852266827100010 16.0596215168986269   T   T   T
 17.5142606545888242  1.3852266827100015 19.6778371195072879   T   T   T
 12.4669534525853027  0.0000000000000011 19.1733194211143285   T   T   T
 15.5845368968761981  0.0000000000000012 20.9973349313652555   T   T   T
 13.6509427783877584  1.3852266827100015 19.6859057901414971   T   T   T
 18.7005602165850036  1.3852266827100008  9.2861208469999994   F   F   F
 18.7005602165850036  0.0000000000000005  8.0000000000000000   F   F   F
 20.5970463633496124  1.3852266827100008  9.2861208469999994   F   F   F
 21.8173202526825030  0.0000000000000005  9.2861208469999994   F   F   F
 21.8173202526825030  1.3852266827100010 12.5708101129999967   F   F   F
 21.8173202526825030  0.0000000000000006 11.2846892659999973   F   F   F
 18.7005602165850036  0.0000000000000006 10.5722416940000006   F   F   F
 23.0375941420153971  1.3852266827100008  9.2861208469999994   F   F   F
 23.7138063994471082  1.3852266827100010 12.5708101129999967   F   F   F
 18.7005602165850036  0.0000000000000007 12.5708101129999967   F   F   F
 18.7005119534225095  1.3852266827100010 15.8817053291980645   T   T   T
 18.7004820764874928  0.0000000000000009 14.6472838646065178   T   T   T
 21.8173202526825030  0.0000000000000008 13.8569309599999961   F   F   F
 19.9208341059178977  1.3852266827100010 12.5708101129999967   F   F   F
 20.5788038867491672  1.3852266827100010 16.0595636794336514   T   T   T
 21.8177320371599883  0.0000000000000009 16.3782699262759017   T   T   T
 21.8183850365613843  1.3852266827100015 19.8128195486280312   T   T   T
 21.8230216886542827  0.0000000000000010 18.2371018241064249   T   T   T
 18.7004790819838540  0.0000000000000010 17.3529530354685022   T   T   T
 23.0556545696761468  1.3852266827100010 16.0566175902512533   T   T   T
 23.7499461529372482  1.3852266827100015 19.6858352116324440   T   T   T
 18.7004475601991835  0.0000000000000011 19.1709128485325664   T   T   T
 21.8162371246063955  0.0000000000000012 20.9972171643965098   T   T   T
 19.8865890386167052  1.3852266827100015 19.6777574256110235   T   T   T

Metal reference: TiO2(110)/fcc(100)_9x1/Pt E_tot= -161.51228425 eV
 D3-zero damping= -12.4015387 eV, D3-BJ damping= -12.993818 eV
Pt
 1.0000000000000000
    24.9340802887800024    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7704533654200003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.0765597851474737
  27
Cartesian
 -0.0000841953088611  0.0000016742003301  8.1033326305899074
  1.3854118259345505  1.3852250758455771 10.0399623559582860
 -0.0000694988810337  0.0000018330801604 11.9762703222138196
  2.7701880591610317 -0.0000055314602360  8.1011268571215407
  4.1554867135175018  1.3852186499340653 10.0379648117761526
  2.7706545252560622 -0.0000049286641637 11.9759881621366944
  5.5408279758618351 -0.0000109583427702  8.1003341395292718
```

```
  6.9258556775701612  1.3852171710788401 10.0374846027473552
  5.5406395912221020  0.0000003956546529 11.9751149944534134
  8.3115120103829572 -0.0000080808160345  8.1007301930006435
  9.6961046721364568  1.3852224089763081 10.0390113436842388
  8.3108088313606654 -0.0000071974295713 11.9756032950960698
 11.0820155925810795 -0.0000008014728561  8.1021912377682455
 12.4669842737491301  1.3852284445521319 10.0399803199770581
 11.0813733468851030 -0.0000001839610895 11.9763588437976889
 13.8519064975514237  0.0000026063632523  8.1019236616778354
 15.2379810634251438  1.3852300960145103 10.0381800964570367
 13.8529976839175841  0.0000033216203572 11.9759900866043427
 16.6227365200592097  0.0000030199973668  8.1003151868387757
 18.0082645260480767  1.3852302450915601 10.0367257662890701
 16.6233767945702766  0.0000034573524748 11.9749914064407204
 19.3933798159430530  0.0000036499569477  8.1001351523626610
 20.7786782929134120  1.3852309328909522 10.0376356823967647
 19.3933898688483666  0.0000037241318770 11.9745603468374622
 22.1639290415469752  0.0000041852308505  8.1008850536189723
 23.5484716262141092  1.3852302842844295 10.0398370271856923
 22.1633251839959904  0.0000041042632595 11.9759006237456749

Interface: TiO2(110)/fcc(100)_9x1/Ir E_tot= -1059.34884483 eV
 D3-zero damping= -30.6787045 eV, D3-BJ damping= -37.7034755 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ir
 1.0000000000000000
    24.4355689309500050    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7150632145500007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.4127819096326846
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2  27
Selective dynamics
Cartesian
  0.0000000000000006  1.3575316072750010  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  8.0000000000000000   F   F   F
  1.8585693728880581  1.3575316072750010  9.2861208469999994   F   F   F
  3.0544461163687515  0.0000000000000005  9.2861208469999994   F   F   F
  3.0544461163687515  1.3575316072750012 12.5708101129999967   F   F   F
  3.0544461163687515  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.2503228598494447  1.3575316072750010  9.2861208469999994   F   F   F
  4.9130154892568090  1.3575316072750012 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000007 12.5708101129999967   F   F   F
 24.4354795259793391  1.3575957365307467 15.9358727528295816   T   T   T
 -0.0000746286023913  0.0000555399049378 14.6293804660478841   T   T   T
  3.0544461163687515  0.0000000000000008 13.8569309599999961   F   F   F
  1.1958767434806938  1.3575316072750012 12.5708101129999967   F   F   F
  1.9349179889971042  1.3574539562051300 16.0418869890134985   T   T   T
  3.2367878495508395 -0.0000780523600937 16.2019659111427217   T   T   T
  3.2418830506769640  1.3575653219247625 19.6090305550355701   T   T   T
  3.2726228619667639 -0.0000006438115903 18.1281083905847389   T   T   T
 24.4355777859683876  0.0000377784554447 17.3722169476640929   T   T   T
  4.5492372925402673  1.3574408854990774 15.8406045420496930   T   T   T
  5.1486718716031392  1.3574648064169179 19.8708283635808591   T   T   T
 -0.0000407552571128 -0.0000017452246138 19.2246246970942885   T   T   T
  3.0880778960489872 -0.0000040027165361 20.9691497118346746   T   T   T
  1.2544437160573974  1.3575574447774321 19.6195927503931138   T   T   T
  6.1088922327375030  1.3575316072750010  9.2861208469999994   F   F   F
  6.1088922327375030  0.0000000000000004  8.0000000000000000   F   F   F
  7.9674616056255587  1.3575316072750010  9.2861208469999994   F   F   F
  9.1633383491062528  0.0000000000000005  9.2861208469999994   F   F   F
  9.1633383491062528  1.3575316072750012 12.5708101129999967   F   F   F
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9.1633383491062528	0.0000000000000006	11.2846892659999973	F	F	F
6.1088922327375030	0.0000000000000006	10.5722416940000006	F	F	F
10.3592150925869451	1.3575316072750010	9.2861208469999994	F	F	F
11.0219077219943120	1.3575316072750012	12.5708101129999967	F	F	F
6.1088922327375030	0.0000000000000007	12.5708101129999967	F	F	F
6.3534014392465838	1.3573572718467224	16.4901026504151496	T	T	T
6.9141295536372702	-0.0001566455307760	15.1629443042594421	T	T	T
9.1633383491062528	0.0000000000000008	13.8569309599999961	F	F	F
7.3047689762181962	1.3575316072750012	12.5708101129999967	F	F	F
8.2421577694841694	1.3573576195962447	16.9386937725887528	T	T	T
8.9307597318909657	-0.0001728424235675	15.7730159672133521	T	T	T
9.1408241206723968	1.3575152144568043	20.4473282396390559	T	T	T
8.4669872869817500	0.0000228947862324	19.2676992251985659	T	T	T
6.1440821639962531	-0.0001552949505838	17.8491742560534945	T	T	T
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10.9347324338452125	1.3577330932055269	19.6831370218134651	T	T	T
6.5142736998474300	0.0000758725087970	19.7873231002764918	T	T	T
9.5785690495731455	0.0000641206795857	21.8267146067928834	T	T	T
7.2341844096230492	1.3575288226064532	21.0050501315181393	T	T	T
12.2177844654750025	1.3575316072750010	9.2861208469999994	F	F	F
12.2177844654750025	0.0000000000000004	8.0000000000000000	F	F	F
14.0763538383630600	1.3575316072750010	9.2861208469999994	F	F	F
15.2722305818437540	0.0000000000000005	9.2861208469999994	F	F	F
15.2722305818437540	1.3575316072750012	12.5708101129999967	F	F	F
15.2722305818437540	0.0000000000000006	11.2846892659999973	F	F	F
12.2177844654750025	0.0000000000000006	10.5722416940000006	F	F	F
16.4681073253244463	1.3575316072750010	9.2861208469999994	F	F	F
17.1307999547318133	1.3575316072750012	12.5708101129999967	F	F	F
12.2177844654750025	0.0000000000000007	12.5708101129999967	F	F	F
12.2176984781699272	1.3573584633291633	15.9012367569691744	T	T	T
12.2177531369499484	-0.0001141251617926	14.5812573806490704	T	T	T
15.2722305818437540	0.0000000000000008	13.8569309599999961	F	F	F
13.4136612089556966	1.3575316072750012	12.5708101129999967	F	F	F
14.1350936530704683	1.3574371597724133	15.8690935474050203	T	T	T
15.5045606612473215	-0.0001189195613540	15.7730149115153360	T	T	T
15.2947335848828025	1.3576190267169408	20.4473840984641733	T	T	T
15.9686285322836721	0.0000905018525917	19.2678173422632355	T	T	T
12.2177514904051385	-0.0001112753104832	17.3711587232350020	T	T	T
16.1932229306846871	1.3574077762254193	16.9386337240277669	T	T	T
17.2014100242414507	1.3576195632167487	21.0051198857614487	T	T	T
12.2177679174064178	0.0002307567052477	19.1996722727769438	T	T	T
14.8567145902103572	0.0000917264269522	21.8266930402057220	T	T	T
13.5008992032230033	1.3577301832643498	19.6829917298230050	T	T	T
18.3266766982125056	1.3575316072750010	9.2861208469999994	F	F	F
18.3266766982125056	0.0000000000000004	8.0000000000000000	F	F	F
20.1852460711005648	1.3575316072750010	9.2861208469999994	F	F	F
21.3811228145812571	0.0000000000000005	9.2861208469999994	F	F	F
21.3811228145812571	1.3575316072750012	12.5708101129999967	F	F	F
21.3811228145812571	0.0000000000000006	11.2846892659999973	F	F	F
18.3266766982125056	0.0000000000000006	10.5722416940000006	F	F	F
22.5769995580619494	1.3575316072750010	9.2861208469999994	F	F	F
23.2396921874693128	1.3575316072750012	12.5708101129999967	F	F	F
18.3266766982125056	0.0000000000000007	12.5708101129999967	F	F	F
18.0820198665236944	1.3573977532912396	16.4900382748540828	T	T	T
17.5213298457621924	-0.0001226452630210	15.1628675021687922	T	T	T
21.3811228145812571	0.0000000000000008	13.8569309599999961	F	F	F
19.5225534416932014	1.3575316072750012	12.5708101129999967	F	F	F
19.8862676605595823	1.3574501171336915	15.8406216603627268	T	T	T
21.1986532465389068	-0.0000703323796422	16.2021651582598025	T	T	T
21.1936251906744388	1.3576092890193650	19.6091639305228504	T	T	T
21.1626906394302736	0.0000514064725926	18.1282181327181604	T	T	T
18.2913117241375573	-0.0000959387176274	17.8491205368357235	T	T	T
22.5005220841539426	1.3574759977572379	16.0420461937234400	T	T	T

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 23.1811107759733837  1.3575712386292189 19.6193983202737634   T   T   T
 17.9213258662790267  0.0000164252954940 19.7872263336765144   T   T   T
 21.3473056507771055  0.0000757860389328 20.9691959538960369   T   T   T
 19.2868736438142214  1.3575453619006990 19.8707953912295459   T   T   T
 -0.0001097794936836 -0.0000414068579906 22.9514420888809347   T   T   T
  1.3839636016768018  1.3574992776048413 24.7714767645967022   T   T   T
 -0.0000851593868123 -0.0000514678312012 26.6300625498565751   T   T   T
  2.8392894108012050 -0.0000030654061661 22.9779133253207561   T   T   T
  4.0653169145092791  1.3575373891133318 24.9954859387997210   T   T   T
  2.6130455914528148 -0.0000257104800727 26.7414962443334332   T   T   T
  5.5466269427563892  0.0000167895269067 23.2685995875403542   T   T   T
  6.7694261057007772  1.3575780201821177 25.2215765572383717   T   T   T
  5.3096463829045986  0.0000161274440976 26.9727095217713781   T   T   T
  8.1975874571478951  0.0000678482750326 23.5013028058866134   T   T   T
  9.5231978257172809  1.3576154317659666 25.4021505531158311   T   T   T
  8.0496713020052262  0.0000729941497834 27.1332909346660678   T   T   T
 10.9173746670075449  0.0000713776880927 23.4764192290135334   T   T   T
 12.2176653447339820  1.3575815642694029 25.3607559704607191   T   T   T
 10.8543499362631461  0.0000837504012891 27.2302150152911047   T   T   T
 13.5179686922461784  0.0000576677594890 23.4764113261268861   T   T   T
 14.9121685559951906  1.3575786780828507 25.4021056429382170   T   T   T
 13.5810360647875736  0.0000559746013352 27.2301660281257227   T   T   T
 16.2377902406727515  0.0000308571549677 23.5012831200869421   T   T   T
 17.6659609435022027  1.3575250603631568 25.2215199404526160   T   T   T
 16.3857113125086045  0.0000011044677408 27.1331985876671276   T   T   T
 18.8887428020625023 -0.0000175300396356 23.2685984227941098   T   T   T
 20.3700394199424863  1.3575036385952033 24.9954992628674901   T   T   T
 19.1257092362628498 -0.0000294515720037 26.9726830073311312   T   T   T
 21.5961252231589569 -0.0000239999172228 22.9779847617789486   T   T   T
 23.0514310129870275  1.3574906642200890 24.7715213779799655   T   T   T
 21.8223671864001751 -0.0000344596220381 26.7415146666046262   T   T   T

Oxide reference: TiO2(110)/fcc(100)_9x1/Ir E_tot= -824.68668391 eV
 D3-zero damping= -14.9593308 eV, D3-BJ damping= -21.7440606 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti
O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
    24.4355689309500050    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7150632145500007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.8017123208283969
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2
4   1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.3575316072750010  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  8.0000000000000000   F   F   F
  1.8585693728880581  1.3575316072750010  9.2861208469999994   F   F   F
  3.0544461163687515  0.0000000000000005  9.2861208469999994   F   F   F
  3.0544461163687515  1.3575316072750012 12.5708101129999967   F   F   F
  3.0544461163687515  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.2503228598494447  1.3575316072750010  9.2861208469999994   F   F   F
  4.9130154892568090  1.3575316072750012 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000007 12.5708101129999967   F   F   F
 24.4355980657604803  1.3575368129939978 15.9517991432809545   T   T   T
  0.0001429445522389  0.0000015183035633 14.6998764346971313   T   T   T
  3.0544461163687515  0.0000000000000008 13.8569309599999961   F   F   F
  1.1958767434806938  1.3575316072750012 12.5708101129999967   F   F   F
  1.8549121810111235  1.3575274997571873 16.2347043974946601   T   T   T
  3.0547843703105215 -0.0000062384706947 16.7324059971310248   T   T   T
  3.0547634894711413  1.3575318464834081 20.1869183391978098   T   T   T
  3.0551994746306206 -0.0000054795321411 18.5580273312283595   T   T   T
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24.4354267150678623	-0.0000191188889183	17.4855975866651789	T	T	T
4.2539676908795583	1.3575258297716768	16.2330346789627420	T	T	T
4.9420818247990441	1.3576052243687939	19.9008629442094254	T	T	T
-0.0000416637527396	0.0000236447003732	19.2999849966136985	T	T	T
3.0548148316763597	0.0000007152537297	21.3909777170821194	T	T	T
1.1673763283496734	1.3575311797772904	19.9006645245552249	T	T	T
6.1088922327375030	1.3575316072750010	9.2861208469999994	F	F	F
6.1088922327375030	0.0000000000000004	8.0000000000000000	F	F	F
7.9674616056255587	1.3575316072750010	9.2861208469999994	F	F	F
9.1633383491062528	0.0000000000000005	9.2861208469999994	F	F	F
9.1633383491062528	1.3575316072750012	12.5708101129999967	F	F	F
9.1633383491062528	0.0000000000000006	11.2846892659999973	F	F	F
6.1088922327375030	0.0000000000000006	10.5722416940000006	F	F	F
10.3592150925869451	1.3575316072750010	9.2861208469999994	F	F	F
11.0219077219943120	1.3575316072750012	12.5708101129999967	F	F	F
6.1088922327375030	0.0000000000000007	12.5708101129999967	F	F	F
6.1090224190530140	1.3575695683364910	15.9512520579366264	T	T	T
6.1089584745718000	-0.0000028528815306	14.6993571128955729	T	T	T
9.1633383491062528	0.0000000000000008	13.8569309599999961	F	F	F
7.3047689762181962	1.3575316072750012	12.5708101129999967	F	F	F
7.9639493209191308	1.3575368749907928	16.2333384829597485	T	T	T
9.1633495639182989	-0.0000096573534050	16.7321724718816043	T	T	T
9.1632412315470795	1.3575332025212943	20.1867218667535049	T	T	T
9.1631503409176922	0.0000007428170120	18.5577307830132021	T	T	T
6.1088336671853130	-0.0000199418961728	17.4851104658133636	T	T	T
10.3629500685670433	1.3575500181804441	16.2340061496995460	T	T	T
11.0505011439800160	1.3575360756304780	19.9006486383495336	T	T	T
6.1090370290496292	0.0000835727144475	19.2995384974727386	T	T	T
9.1630917328178416	0.0000021312928251	21.3907357072013298	T	T	T
7.2761678631773821	1.3576052091574000	19.9004133119388840	T	T	T
12.2177844654750025	1.3575316072750010	9.2861208469999994	F	F	F
12.2177844654750025	0.0000000000000004	8.0000000000000000	F	F	F
14.0763538383630600	1.3575316072750010	9.2861208469999994	F	F	F
15.2722305818437540	0.0000000000000005	9.2861208469999994	F	F	F
15.2722305818437540	1.3575316072750012	12.5708101129999967	F	F	F
15.2722305818437540	0.0000000000000006	11.2846892659999973	F	F	F
12.2177844654750025	0.0000000000000006	10.5722416940000006	F	F	F
16.4681073253244463	1.3575316072750010	9.2861208469999994	F	F	F
17.1307999547318133	1.3575316072750012	12.5708101129999967	F	F	F
12.2177844654750025	0.0000000000000007	12.5708101129999967	F	F	F
12.2178024856220322	1.3575896552707378	15.9516300690635902	T	T	T
12.2178428487752804	0.0000608063616421	14.6997745278659515	T	T	T
15.2722305818437540	0.0000000000000008	13.8569309599999961	F	F	F
13.4136612089556966	1.3575316072750012	12.5708101129999967	F	F	F
14.0726179284974560	1.3575613393168580	16.2345202304331906	T	T	T
15.2723491617456713	0.0000198193834018	16.7323540819032708	T	T	T
15.2724060597576550	1.3575225988421746	20.1868512492495853	T	T	T
15.2727653305889266	0.0000043162975496	18.5579083556054947	T	T	T
12.2176787691667492	0.0000636321739950	17.4855532513634131	T	T	T
16.4716172130072245	1.3575564785879857	16.2331829501265261	T	T	T
17.1594906614922174	1.3575245004655425	19.9008589498764650	T	T	T
12.2177891532439897	0.0000055915202133	19.2999119752981940	T	T	T
15.2724113628910736	-0.0000049863126919	21.3908780357055690	T	T	T
13.3851817669754674	1.3575345900253022	19.9004319828844629	T	T	T
18.3266766982125056	1.3575316072750010	9.2861208469999994	F	F	F
18.3266766982125056	0.0000000000000004	8.0000000000000000	F	F	F
20.1852460711005648	1.3575316072750010	9.2861208469999994	F	F	F
21.3811228145812571	0.0000000000000005	9.2861208469999994	F	F	F
21.3811228145812571	1.3575316072750012	12.5708101129999967	F	F	F
21.3811228145812571	0.0000000000000006	11.2846892659999973	F	F	F
18.3266766982125056	0.0000000000000006	10.5722416940000006	F	F	F
22.5769995580619494	1.3575316072750010	9.2861208469999994	F	F	F
23.2396921874693128	1.3575316072750012	12.5708101129999967	F	F	F

```
 18.3266766982125056  0.0000000000000007 12.5708101129999967   F   F   F
 18.3265705121812523  1.3574677928970211 15.9512246125528776   T   T   T
 18.3267211228624802 -0.0000159750637757 14.6993331284560256   T   T   T
 21.3811228145812571  0.0000000000000008 13.8569309599999961   F   F   F
 19.5225534416932014  1.3575316072750012 12.5708101129999967   F   F   F
 20.1815754297880012  1.3575508736719728 16.2332488355918976   T   T   T
 21.3808977142146830  0.0000404699163186 16.7322305621650322   T   T   T
 21.3808062342184115  1.3575278885521003 20.1868249401396760   T   T   T
 21.3807155891306309  0.0000041454851067 18.5578745557997742   T   T   T
 18.3265627423417854 -0.0000284704022624 17.4850936145322073   T   T   T
 22.5806588959215553  1.3575468903673720 16.2342248119249710   T   T   T
 23.2682692071876396  1.3575294324890934 19.9010215365551559   T   T   T
 18.3263805552823449 -0.0000144995434271 19.2995267989625212   T   T   T
 21.3806293781968364 -0.0000001165925094 21.3908594099246017   T   T   T
 19.4935185264016440  1.3575225191768860 19.9005106827990268   T   T   T

Metal reference: TiO2(110)/fcc(100)_9x1/Ir E_tot= -226.25354521 eV
 D3-zero damping= -11.1633294 eV, D3-BJ damping= -12.1000406 eV
Ir
 1.0000000000000000
    24.4355689309500050    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7150632145500007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.0765597851474737
  27
Cartesian
  0.0000225822385718 -0.0000013302660664  8.1850145846723734
  1.3567702455022848  1.3575301249344049 10.0391515899893413
 -0.0000205079539215 -0.0000018370209633 11.8926969122899155
  2.7129940440779317 -0.0000016138150602  8.1837766610392091
  4.0716476681621225  1.3575304326792494 10.0353081046880703
  2.7161824233696450 -0.0000001366149545 11.8909469685019822
  5.4306372139803587  0.0000014403611109  8.1842516029975148
  6.7873613675378692  1.3575325198706791 10.0383719081877594
  5.4283200588542186 -0.0000004075777783 11.8899641405747118
  8.1463582404346351  0.0000005679350461  8.1854918290280931
  9.5024215374170229  1.3575329039600808 10.0399469821597638
  8.1442371958854096  0.0000034099476916 11.8925436905430590
 10.8605230719954520  0.0000022834977765  8.1866175637744956
 12.2177894429999228  1.3575328436207890 10.0408008214614615
 10.8596474045994817  0.0000018737839495 11.8939695912072807
 13.5750394385765638  0.0000002882479106  8.1866236268679877
 14.9331965031104623  1.3575328768095971 10.0399169766169241
 13.5759376929348718  0.0000031894974760 11.8939417802869265
 16.2892047854243813  0.0000009298871012  8.1854463679244329
 17.6482371170153485  1.3575311173094164 10.0382795000739318
 16.2913679363919108 -0.0000007847733145 11.8924881391124249
 19.0049522644336228 -0.0000021868000364  8.1841478278818123
 20.3638832705548438  1.3575310660984112 10.0352217382759399
 19.0072580838266632 -0.0000009523391510 11.8899004826894519
 21.7226099316404486 -0.0000015408737031  8.1837475387362506
 23.0788007777677429  1.3575299539980528 10.0391142162075440
 21.7193676323392282 -0.0000021721330612 11.8908544468175847

Interface: ZnO(11-20)/fcc(100)_2x2/Au E_tot= -111.20821068 eV
 D3-zero damping= -9.0935082 eV, D3-BJ damping= -8.6439116 eV
Zn  O Zn  O Zn  O Zn  O Au
 1.0000000000000000
     5.7975034209400009    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7975034209400009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.5844023453527321
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
```

```
  3.8651475864454046  0.0054219282748112  8.0000000000000000   F   F   F
  1.9326455429736991  2.9041736448799096  8.0000055199296671   F   F   F
  3.8651474755987283  2.2034268672626758  8.0000008619369254   F   F   F
  1.9326462778270093  5.1021785872831265  8.0000049280612373   F   F   F
  0.9663903176525029  0.0054219494837394  9.6370125635575068   F   F   F
  4.8313916951207991  2.9041736660888375  9.6370180834871757   F   F   F
  0.9663902068058258  2.2034268884716037  9.6370134254944340   F   F   F
  4.8313924299741080  5.1021786084920544  9.6370174916187459   F   F   F
  3.8464897416920270  0.1092909642669857 11.2462877066959610   T   T   T
  1.9513033783370921  3.0081203321130818 11.2461740975107087   T   T   T
  3.7831628550829124  2.1534590099219106 11.2271023729178427   T   T   T
  2.0147686384903665  5.0521718432657963 11.2270353018710090   T   T   T
  0.9582049051576231  0.1283226002399942 12.6365150558644803   T   T   T
  4.8397614182524720  3.0271178583624159 12.6362183852579566   T   T   T
  0.8162644173245412  2.0813469989317470 12.5773541407206988   T   T   T
  4.9817950779987337  4.9801553481467140 12.5772636115982426   T   T   T
  0.0082415825096123 -0.8181948693368212 14.9146376657299928   T   T   T
  1.4917450540131425  0.6376052066957377 16.8404353740193145   T   T   T
  0.0102799805966129 -0.8173718455708636 18.9282889250669939   T   T   T
 -0.0079741750890935  2.0804106426503792 14.9147476960411574   T   T   T
  1.4790837062823785  3.5296656498417458 16.8661506618944657   T   T   T
 -0.0102938854036541  2.0813730005312174 18.9283481330740919   T   T   T
  2.8626734610978746 -0.7957356865080856 14.6163622117774494   T   T   T
  4.3183254367000625  0.6309524671873370 16.8659841823166659   T   T   T
  2.8996321909271994 -0.8178016789873980 18.9445817414883955   T   T   T
  2.9350028018154322  2.1030505810320816 14.6164829021904197   T   T   T
  4.3056914993975299  3.5365164533886424 16.8401096897655869   T   T   T
  2.8980886432253099  2.0810979001644063 18.9445620748411869   T   T   T

Oxide reference: ZnO(11-20)/fcc(100)_2x2/Au E_tot= -68.46796372 eV
 D3-zero damping= -2.0171489 eV, D3-BJ damping= -2.1785158 eV
Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     5.7975034209400009    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7975034209400009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.8298334931259674
   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.8651475864454046  0.0054219282748112  8.0000000000000000   F   F   F
  1.9326455429736991  2.9041736448799096  8.0000055199296689   F   F   F
  3.8651474755987283  2.2034268672626758  8.0000008619369254   F   F   F
  1.9326462778270093  5.1021785872831265  8.0000049280612373   F   F   F
  0.9663903176525029  0.0054219494837394  9.6370125635575086   F   F   F
  4.8313916951207991  2.9041736660888375  9.6370180834871775   F   F   F
  0.9663902068058258  2.2034268884716037  9.6370134254944340   F   F   F
  4.8313924299741080  5.1021786084920544  9.6370174916187459   F   F   F
  3.8094092527731958  0.1069963271727204 11.2604992420086703   T   T   T
  1.9882563800399904  3.0057723717115823 11.2606247670865294   T   T   T
  3.8387106460726823  2.1967970762690108 11.2785545480346681   T   T   T
  1.9589353218588372  5.0955391423931449 11.2785661105956958   T   T   T
  0.6998524472887615  0.2978541278593533 12.4825451261662135   T   T   T
  5.0976509993217629  3.1966077180664514 12.4827176793508841   T   T   T
  0.8982348880501140  2.1686858172197714 12.6984500697764577   T   T   T
  4.8992298128569693  5.0674574565856521 12.6984169703822509   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_2x2/Au E_tot= -39.96243399 eV
 D3-zero damping= -4.9247509 eV, D3-BJ damping= -4.971358 eV
Au
 1.0000000000000000
     5.7975034209400009    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7975034209400009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7797100266724897
```

```
  12
Cartesian
 -0.0000003453694479 -0.0000008186720787  7.8114080449387160
  1.4493731611863152  1.4493751355809514  9.8898972223209700
 -0.0000004319210546 -0.0000004024066548 11.9677685183251228
 -0.0000003051801963  2.8987521234044302  7.8114091455120853
  1.4493730728869916  4.3481283408964302  9.8898975606266593
 -0.0000004990108040  2.8987522320534995 11.9677705711882378
  2.8987520471420241 -0.0000007158407110  7.8114074924325250
  4.3481303257475536  1.4493751012091236  9.8898977050694690
  2.8987520970187961 -0.0000003716462074 11.9677688548822694
  2.8987521576063200  2.8987522665984149  7.8114087002934962
  4.3481303764851118  4.3481282320905237  9.8898981618870039
  2.8987520611110051  2.8987522109579440 11.9677695883931499

Interface: ZnO(11-20)/fcc(100)_2x2/Ag E_tot= -104.17771443 eV
 D3-zero damping= -7.6057507 eV, D3-BJ damping= -8.1601502 eV
Zn  O Zn  O Zn  O Zn  O Ag
 1.0000000000000000
     5.7610541039000012    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7610541039000012    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.5844023453527321
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.8408471282040368  0.0053878402254721  8.0000000000000000   F   F   F
  1.9204948627572189  2.8859148982719987  8.0000055199296671   F   F   F
  3.8408470180542613  2.1895737655690697  8.0000008619369254   F   F   F
  1.9204955929904539  5.0701008270094761  8.0000049280612373   F   F   F
  0.9603145528767072  0.0053878613010583  9.6370125635575068   F   F   F
  4.8010163913298909  2.8859149193475844  9.6370180834871757   F   F   F
  0.9603144427269310  2.1895737866446554  9.6370134254944340   F   F   F
  4.8010171215631248  5.0701008480850618  9.6370174916187459   F   F   F
  3.8161457112018256  0.1016076839869368 11.2455553526923300   T   T   T
  1.9450465491607147  2.9821655645300464 11.2456559926254176   T   T   T
  3.7826584213395433  2.1437855026520465 11.2430245116839451   T   T   T
  1.9787292211680114  5.0241863934800355 11.2430207425891897   T   T   T
  0.9103185973910903  0.1272694967832790 12.6488298785795177   T   T   T
  4.8506713904198007  3.0077764234410673 12.6490155554884538   T   T   T
  0.8769446595092785  2.0963438117401347 12.6671324405529671   T   T   T
  4.8837778454436256  4.9767596230563917 12.6677869414240281   T   T   T
  0.0582543615166841 -1.0507257734054396 14.9107950329675401   T   T   T
  1.4927874937433578  0.4105914380445745 16.7983206431607854   T   T   T
  0.0026494077328188 -1.0335058960408428 18.8568557491644739   T   T   T
 -0.0544124063601838  1.8300349302435928 14.9104714899585602   T   T   T
  1.4767618505388282  3.2839452659790971 16.8350853706221031   T   T   T
  0.0000735918169364  1.8470835235092300 18.8567474518061076   T   T   T
  2.9159855838757802 -0.9770176363372876 14.5763626077708928   T   T   T
  4.2874287244709990  0.4034727364048733 16.8347896243162189   T   T   T
  2.8761668143321053 -1.0325045063868881 18.9020740962691534   T   T   T
  2.8482072962338165  1.9034900047824062 14.5767329764390023   T   T   T
  4.2714256635891328  3.2912189407154946 16.7984013693321295   T   T   T
  2.8877409899545667  1.8481204585051523 18.9022940497028884   T   T   T

Oxide reference: ZnO(11-20)/fcc(100)_2x2/Ag E_tot= -68.66785485 eV
 D3-zero damping= -2.0281952 eV, D3-BJ damping= -2.201637 eV
Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     5.7610541039000012    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7610541039000012    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.8298334931259674
   2   2   2   2   2   2   2   2
Selective dynamics
```

```
Cartesian
  3.8408471282040368  0.0053878402254721  8.0000000000000000   F   F   F
  1.9204948627572189  2.8859148982719987  8.0000055199296689   F   F   F
  3.8408470180542613  2.1895737655690697  8.0000008619369254   F   F   F
  1.9204955929904539  5.0701008270094761  8.0000049280612373   F   F   F
  0.9603145528767072  0.0053878613010583  9.6370125635575086   F   F   F
  4.8010163913298909  2.8859149193475844  9.6370180834871775   F   F   F
  0.9603144427269310  2.1895737866446554  9.6370134254944340   F   F   F
  4.8010171215631248  5.0701008480850618  9.6370174916187459   F   F   F
  3.7860286496791957  0.1067701545267709 11.2651622696599265   T   T   T
  1.9752067155250910  2.9872876599405411 11.2652330658001851   T   T   T
  3.8209238212297909  2.1826665017529119 11.2822823745306557   T   T   T
  1.9403713296123137  5.0632302150416795 11.2822814031569951   T   T   T
  0.6982650674537424  0.2949366268777738 12.5044400842183308   T   T   T
  5.0629685373852835  3.1754366453762546 12.5044832788404285   T   T   T
  0.9068601146262028  2.1615274249945506 12.7220305965827922   T   T   T
  4.8544627572418788  5.0420609138796522 12.7219956576514903   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_2x2/Ag E_tot= -32.65814595 eV
 D3-zero damping= -3.5931606 eV, D3-BJ damping= -4.5228221 eV
Ag
 1.0000000000000000
     5.7610541039000012    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.7610541039000012    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7797100266724897
  12
Cartesian
 -0.0000007465418771 -0.0000012713148150  7.8238030436730206
  1.4402600782529711  1.4402625046914181  9.8900299518424202
 -0.0000008413529930 -0.0000009229109768 11.9552423208712124
 -0.0000007262337309  2.8805279384216473  7.8238023006778734
  1.4402599436972876  4.3207916075604453  9.8900300349973431
 -0.0000009722344152  2.8805280932885506 11.9552421530225050
  2.8805277133898839 -0.0000011388377251  7.8238019336226898
  4.3207941367789182  1.4402625961036482  9.8900302126846089
  2.8805279563999595 -0.0000009361932129 11.9552435535336201
  2.8805276887100577  2.8805280320795514  7.8238011006277111
  4.3207942328020721  4.3207914023634277  9.8900307559859666
  2.8805280474408597  2.8805281018839541 11.9552440260539310

Interface: ZnO(11-20)/fcc(100)_2x2/Cu E_tot= -114.67031555 eV
 D3-zero damping= -7.3448073 eV, D3-BJ damping= -8.6308999 eV
Zn  O Zn  O Zn  O Zn  O Cu
 1.0000000000000000
     5.0475392734600009    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.0475392734600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.5844023453527321
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.3651526913871259  0.0047205484702510  8.0000000000000000   F   F   F
  1.6826388139078479  2.5284901905417141  8.0000055199296671   F   F   F
  3.3651525948795586  1.9183919078916216  8.0000008619369254   F   F   F
  1.6826394537006473  4.4421615529366276  8.0000049280612373   F   F   F
  0.8413782153580166  0.0047205669355955  9.6370125635575068   F   F   F
  4.2064036113387395  2.5284902090070580  9.6370180834871757   F   F   F
  0.8413781188504484  1.9183919263569660  9.6370134254944340   F   F   F
  4.2064042511315387  4.4421615714019724  9.6370174916187459   F   F   F
  3.4808251524807341 -0.0613573411045807 11.4346066402490152   T   T   T
  1.5686465752460617  2.4624743999559522 11.4340398014806421   T   T   T
  3.4717074391680041  1.9137250541848869 11.4102565764734329   T   T   T
  1.5774645410688812  4.4377087908694985 11.4099881743866778   T   T   T
  1.0151576415099883 -0.0718734896511317 13.2072660716310981   T   T   T
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```
  4.0351685979293022  2.4514952870816686 13.2075875307802786   T   T   T
  0.9857085438298951  1.9106460972673203 13.2457071558591828   T   T   T
  4.0640582673240981  4.4341373221453155 13.2460419404669629   T   T   T
  0.0393912663431366 -0.9974669758083953 15.2397832224512388   T   T   T
  1.2947365531877302  0.2888746051171454 16.9319188219560246   T   T   T
  0.0008993400705931 -0.9681613090044804 18.7077127839575041   T   T   T
 -0.0332572081031090  1.5264675625589352 15.2392681248245214   T   T   T
  1.2866687399066554  2.8223226464046007 16.9509761022971936   T   T   T
  0.0045495513557834  1.5555595297776954 18.7077252030035233   T   T   T
  2.5819091180069691 -0.9178737334538701 15.0402589914890168   T   T   T
  3.7668121954278551  0.2985262993330234 16.9507636197609663   T   T   T
  2.5272776175193403 -0.9678234892805218 18.7359297147946577   T   T   T
  2.4715157279263780  1.6057113085310297 15.0415822330650943   T   T   T
  3.7587700179259622  2.8127407953541015 16.9318477374064393   T   T   T
  2.5258822197930293  1.5559124698681597 18.7360040983509997   T   T   T

Oxide reference: ZnO(11-20)/fcc(100)_2x2/Cu E_tot= -68.37949268 eV
 D3-zero damping= -2.3634577 eV, D3-BJ damping= -2.7120133 eV
Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     5.0475392734600009    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.0475392734600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.8298334931259674
   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.3651526913871259  0.0047205484702510  8.0000000000000000   F   F   F
  1.6826388139078479  2.5284901905417141  8.0000055199296689   F   F   F
  3.3651525948795586  1.9183919078916216  8.0000008619369254   F   F   F
  1.6826394537006473  4.4421615529366276  8.0000049280612373   F   F   F
  0.8413782153580166  0.0047205669355955  9.6370125635575086   F   F   F
  4.2064036113387395  2.5284902090070580  9.6370180834871775   F   F   F
  0.8413781188504484  1.9183919263569660  9.6370134254944340   F   F   F
  4.2064042511315387  4.4421615714019724  9.6370174916187459   F   F   F
  3.4431380527133801 -0.0608008823683358 11.4466460737196734   T   T   T
  1.6047391081215370  2.4630540461025414 11.4465772679986255   T   T   T
  3.4936842649383837  1.9150542139724622 11.4176615953552201   T   T   T
  1.5541910615484886  4.4388445476569602 11.4176182896999929   T   T   T
  0.7696924444505379  0.1111745891708898 13.0757191610742556   T   T   T
  4.2781292072255050  2.6348283910006276 13.0758460749064387   T   T   T
  1.0268512443869113  1.9741077738447199 13.2798713560365886   T   T   T
  4.0211003706038895  4.4978235108081144 13.2799150740795877   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_2x2/Cu E_tot= -43.47721604 eV
 D3-zero damping= -3.4281096 eV, D3-BJ damping= -4.3400294 eV
Cu
 1.0000000000000000
     5.0475392734600009    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.0475392734600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7797100266724897
  12
Cartesian
 -0.0000008261175003 -0.0000013473553495  8.0931417867388280
  1.2618815367452108  1.2618838952552278  9.8899771257775466
 -0.0000011737367894 -0.0000015420644981 11.6859549754694427
 -0.0000007958035477  2.5237708622970825  8.0931430770439299
  1.2618815790142799  3.7856554265578488  9.8899770006934489
 -0.0000011845872811  2.5237710386485244 11.6859573941104227
  2.5237705728004842 -0.0000014225192413  8.0931411079036994
  3.7856576883615087  1.2618838044333818  9.8899772489618218
  2.5237709058810469 -0.0000013271874450 11.6859553197042523
  2.5237705685691494  2.5237709443553209  8.0931424787571782
  3.7856578259791496  3.7856554051663123  9.8899773931145916
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  2.5237708270577448  2.5237710587003757 11.6859561425974405

Interface: ZnO(11-20)/fcc(100)_2x2/Pt E_tot= -144.84782517 eV
 D3-zero damping= -9.9102263 eV, D3-BJ damping= -9.8572088 eV
Zn  O Zn  O Zn  O Zn  O Pt
 1.0000000000000000
     5.5409067308400006    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.5409067308400006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.5844023453527321
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.6940766951635347  0.0051819544881204  8.0000000000000000   F   F   F
  1.8471069216988256  2.7756353257716802  8.0000055199296671   F   F   F
  3.6940765892229166  2.1059035024682924  8.0000008619369254   F   F   F
  1.8471076240276312  4.8763568770160415  8.0000049280612373   F   F   F
  0.9236180174312270  0.0051819747583444  9.6370125635575068   F   F   F
  4.6175549748065192  2.7756353460419034  9.6370180834871757   F   F   F
  0.9236179114906082  2.1059035227385166  9.6370134254944340   F   F   F
  4.6175556771353241  4.8763568972862661  9.6370174916187459   F   F   F
  3.8248819488840584  0.0974523078821769 11.3347025157670629   T   T   T
  1.7166207687848409  2.8679960713244461 11.3345255057737226   T   T   T
  3.5495572595636755  2.0584347430318650 11.2008523483519262   T   T   T
  1.9919107892787793  4.8290222488393146 11.2006992240552190   T   T   T
  1.3078310680894389  0.0877759550483020 12.8185685311515947   T   T   T
  4.2337192880466041  2.8583725952442780 12.8185617241157939   T   T   T
  0.6034412478691283  1.9387529364105289 12.6818426341257489   T   T   T
  4.9382284075719509  4.7093163276369259 12.6819416728395975   T   T   T
 -0.0940953632245233 -0.7088424535484522 14.7737565921691960   T   T   T
  1.3668309576475830  0.5994818370937698 16.7853293401838286   T   T   T
 -0.0207587006538818 -0.7905138484907426 18.7444218451188434   T   T   T
  0.0947463210901314  2.0616484551480383 14.7735663230908152   T   T   T
  1.3809407643222098  3.3923003826675950 16.8026662071132193   T   T   T
  0.0209363201313677  1.9799737259199401 18.7447317245277034   T   T   T
  2.7157080110506855 -0.7624341100975393 14.8347507057212180   T   T   T
  4.1600654180866021  0.6218270942710551 16.8023134482912297   T   T   T
  2.7693939534882150 -0.7936264870037613 18.7370767160893159   T   T   T
  2.8255015881651695  2.0082234047404763 14.8348914865777513   T   T   T
  4.1742132911016903  3.3698766441134551 16.7854256653957492   T   T   T
  2.7715759382779530  1.9767393362958872 18.7367012084510947   T   T   T

Oxide reference: ZnO(11-20)/fcc(100)_2x2/Pt E_tot= -69.46848932 eV
 D3-zero damping= -2.0987568 eV, D3-BJ damping= -2.3429909 eV
Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     5.5409067308400006    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.5409067308400006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.8298334931259674
   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.6940766951635347  0.0051819544881204  8.0000000000000000   F   F   F
  1.8471069216988256  2.7756353257716802  8.0000055199296689   F   F   F
  3.6940765892229166  2.1059035024682924  8.0000008619369254   F   F   F
  1.8471076240276312  4.8763568770160415  8.0000049280612373   F   F   F
  0.9236180174312270  0.0051819747583444  9.6370125635575086   F   F   F
  4.6175549748065192  2.7756353460419034  9.6370180834871775   F   F   F
  0.9236179114906082  2.1059035227385166  9.6370134254944340   F   F   F
  4.6175556771353241  4.8763568972862661  9.6370174916187459   F   F   F
  3.6635881331665736  0.0692405690046380 11.3096131194675547   T   T   T
  1.8776120975982735  2.8397130762511797 11.3096336291861643   T   T   T
  3.7170864757136157  2.0897543191130485 11.3126129791754142   T   T   T
  1.8240644077685926  4.8602310384295579 11.3126388631050858   T   T   T
```

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  0.6970043818927175  0.2421685545180084 12.6631123587063747   T   T   T
  4.8440353042216060  3.0126523098715672 12.6631171653458452   T   T   T
  0.9526520450888910  2.0920868891545137 12.8891820175777454   T   T   T
  4.5884336913917476  4.8625427338110869 12.8892100581536422   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_2x2/Pt E_tot= -71.75552136 eV
 D3-zero damping= -5.51181 eV, D3-BJ damping= -5.775086 eV
Pt
 1.0000000000000000
     5.5409067308400006    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.5409067308400006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7797100266724897
  12
Cartesian
 -0.0000000205343444 -0.0000003947876435  7.9518410331813589
  1.3852241433129404  1.3852259437439070  9.8898978992605784
 -0.0000000191341811  0.0000000865127984 11.8273325078594365
 -0.0000000015509259  2.7704533587687621  7.9518442119248451
  1.3852240698417331  4.1556807196969370  9.8898982070605310
 -0.0000000753264046  2.7704533928092965 11.8273391477934879
  2.7704534052679350 -0.0000002360711666  7.9518390841063669
  4.1556826093148640  1.3852259631307742  9.8898981981120269
  2.7704533688161619  0.0000000737381169 11.8273331544247036
  2.7704533958247461  2.7704534488477131  7.9518442897764343
  4.1556826159149480  4.1556806976069458  9.8898986883467490
  2.7704534327544184  2.7704534148210995 11.8273349822112266

Interface: ZnO(11-20)/fcc(100)_2x2/Pd E_tot= -133.92581529 eV
 D3-zero damping= -8.2574943 eV, D3-BJ damping= -8.9582606 eV
Zn  O Zn  O Zn  O Zn  O Pd
 1.0000000000000000
     5.4959624638000006    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4959624638000006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.5844023453527321
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.6641127240088527  0.0051399218105070  8.0000000000000000   F   F   F
  1.8321243798924092  2.7531211595265050  8.0000055199296671   F   F   F
  3.6641126189275570  2.0888217694644493  8.0000008619369254   F   F   F
  1.8321250765243757  4.8368030104181603  8.0000049280612373   F   F   F
  0.9161262228866016  0.0051399419163120  9.6370125635575068   F   F   F
  4.5801003425701587  2.7531211796323096  9.6370180834871757   F   F   F
  0.9161261178053050  2.0888217895702543  9.6370134254944340   F   F   F
  4.5801010392021242  4.8368030305239653  9.6370174916187459   F   F   F
  3.7113864407612587  0.0739723070172211 11.3138433836724133   T   T   T
  1.7849450040517671  2.8219769413921578 11.3137859219360202   T   T   T
  3.6242746239791224  2.0568243888108850 11.2624235588453168   T   T   T
  1.8719919483999843  4.8048261392460114 11.2623949608106813   T   T   T
  1.0645186813123215  0.0697989822065157 12.8621733226885677   T   T   T
  4.4317376800211408  2.8178181943674843 12.8622365148844917   T   T   T
  0.8539424069718144  2.0238367002460151 12.8532280458244017   T   T   T
  4.6420042035964473  4.7719135577849032 12.8536895349193063   T   T   T
 -0.0012224316508752 -0.8393203183066993 14.9365959904555865   T   T   T
  1.4040272596128491  0.5580635505150864 16.8322281787915777   T   T   T
 -0.0071919000671555 -0.8084596933666345 18.7660637772286698   T   T   T
  0.0022860757359549  1.9086526840706517 14.9364887733013365   T   T   T
  1.3970463554130563  3.3239060242414160 16.8207566529702461   T   T   T
  0.0078919003346953  1.9394953108828701 18.7661508816085103   T   T   T
  2.7361099049389521 -0.7843597045742036 14.7525516630446010   T   T   T
  4.0996595283747643  0.5758703008012638 16.8206460414685210   T   T   T
  2.7607422727312434 -0.8042450241600123 18.7989486337601939   T   T   T
  2.7608424178051374  1.9635367976169238 14.7527903577456510   T   T   T
```

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  4.0927901624898348  3.3061054931002936 16.8320561553190018   T   T   T
  2.7363409887148959  1.9437515994635226 18.7988318726101120   T   T   T

Oxide reference: ZnO(11-20)/fcc(100)_2x2/Pd E_tot= -69.54718879 eV
 D3-zero damping= -2.1154506 eV, D3-BJ damping= -2.3735898 eV
Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     5.4959624638000006    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4959624638000006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.8298334931259674
   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.6641127240088527  0.0051399218105070  8.0000000000000000   F   F   F
  1.8321243798924092  2.7531211595265050  8.0000055199296689   F   F   F
  3.6641126189275570  2.0888217694644493  8.0000008619369254   F   F   F
  1.8321250765243757  4.8368030104181603  8.0000049280612373   F   F   F
  0.9161262228866016  0.0051399419163120  9.6370125635575086   F   F   F
  4.5801003425701587  2.7531211796323096  9.6370180834871775   F   F   F
  0.9161261178053050  2.0888217895702543  9.6370134254944340   F   F   F
  4.5801010392021242  4.8368030305239653  9.6370174916187459   F   F   F
  3.6408051155061902  0.0601772962199809 11.3198843332393029   T   T   T
  1.8552964567696135  2.8081761103651055 11.3199164396299619   T   T   T
  3.6962732285720556  2.0730055371070324 11.3199179427363372   T   T   T
  1.7998339578849680  4.8210079791399254 11.3199813588302671   T   T   T
  0.6993582848252859  0.2340580177039805 12.6958913011067782   T   T   T
  4.7966545677032588  2.9820292994218920 12.6958649753072645   T   T   T
  0.9601679662841429  2.0815053196425417 12.9251495756618482   T   T   T
  4.5358617513609012  4.8294649530244937 12.9251847116541523   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_2x2/Pd E_tot= -60.89865578 eV
 D3-zero damping= -4.0782854 eV, D3-BJ damping= -4.9824562 eV
Pd
 1.0000000000000000
     5.4959624638000006    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4959624638000006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7797100266724897
  12
Cartesian
 -0.0000003363454922 -0.0000007183144019  7.9360296630788065
  1.3739879591383273  1.3739900461449273  9.8899201056603196
 -0.0000004560528752 -0.0000003270204121 11.8431226831156735
 -0.0000003242290864  2.7479817081437212  7.9360316202720220
  1.3739878761558635  4.1219724560033066  9.8899202636511703
 -0.0000005360741181  2.7479816718986045 11.8431274817963104
  2.7479815573817716 -0.0000005817759680  7.9360284098228782
  4.1219745771840399  1.3739900607024300  9.8899203755425891
  2.7479816357317493 -0.0000003459061060 11.8431238584512517
  2.7479815272474628  2.7479816827858188  7.9360315119881433
  4.1219746081383191  4.1219723335639138  9.8899207487235277
  2.7479816038120535  2.7479816999464988 11.8431242712426332

Interface: ZnO(11-20)/fcc(100)_2x2/Ni E_tot= -131.8885697 eV
 D3-zero damping= -6.5625784 eV, D3-BJ damping= -7.7481401 eV
Zn  O Zn  O Zn  O Zn  O Ni
 1.0000000000000000
     4.9077161635400008    0.0000000000000000    0.0000000000000000
     0.0000000000000000    4.9077161635400008    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.5844023453527321
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.2719337803150639  0.0045897834118969  8.0000000000000000   F   F   F
```

```
  1.6360276279246586  2.4584478703753945  8.0000055199296671   F   F   F
  3.2719336864808763  1.8652500682595550  8.0000008619369254   F   F   F
  1.6360282499944023  4.3191081581142248  8.0000049280612373   F   F   F
  0.8180709933005536  0.0045898013657284  9.6370125635575068   F   F   F
  4.0898810044501488  2.4584478883292258  9.6370180834871757   F   F   F
  0.8180708994663650  1.8652500862133865  9.6370134254944340   F   F   F
  4.0898816265198921  4.3191081760680561  9.6370174916187459   F   F   F
  3.4289660997062272 -0.0960267769913235 11.4927510129175836   T   T   T
  1.4790500677806400  2.3577239863248560 11.4927732554951039   T   T   T
  3.4132730573747767  1.8814293224269625 11.4573653851475239   T   T   T
  1.4947493020381910  4.3351697252744001 11.4573576182362089   T   T   T
  1.0642435797838927 -0.0858820899023260 13.3028325666251348   T   T   T
  3.8439697945254272  2.3680606827671062 13.3028198986607435   T   T   T
  1.0337707063819033  1.9035775719960348 13.4099659892675085   T   T   T
  3.8741826262153354  4.3574765184129349 13.4101270851205516   T   T   T
  0.0137504850037331 -0.8226099514836449 15.2964780079017828   T   T   T
  1.2446859369350920  0.4086221747039773 16.9889557782737555   T   T   T
 -0.0026626135017350 -0.8067975714203535 18.6838822575173644   T   T   T
 -0.0131300444589686  1.6308837769007265 15.2963759405735669   T   T   T
  1.2435983956974381  2.8941259236558627 16.9787530067704537   T   T   T
  0.0031252766821062  1.6472637195672970 18.6837622774197492   T   T   T
  2.5053677919684505 -0.7643804025891003 15.1549666594343950   T   T   T
  3.6644661629484325  0.4400458092286864 16.9787801835578698   T   T   T
  2.4589192216368816 -0.8123006118518614 18.7023992517133237   T   T   T
  2.4029681320402974  1.6891608187675549 15.1552278090604684   T   T   T
  3.6633168480294036  2.8624580284707029 16.9886688720472350   T   T   T
  2.4487777690936445  1.6415776069347536 18.7024478156635503   T   T   T

Oxide reference: ZnO(11-20)/fcc(100)_2x2/Ni E_tot= -67.13984677 eV
 D3-zero damping= -2.4655693 eV, D3-BJ damping= -2.8302051 eV
Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     4.9077161635400008    0.0000000000000000    0.0000000000000000
     0.0000000000000000    4.9077161635400008    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.8298334931259674
   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.2719337803150639  0.0045897834118969  8.0000000000000000   F   F   F
  1.6360276279246586  2.4584478703753945  8.0000055199296689   F   F   F
  3.2719336864808763  1.8652500682595550  8.0000008619369254   F   F   F
  1.6360282499944023  4.3191081581142248  8.0000049280612373   F   F   F
  0.8180709933005536  0.0045898013657284  9.6370125635575086   F   F   F
  4.0898810044501488  2.4584478883292258  9.6370180834871775   F   F   F
  0.8180708994663650  1.8652500862133865  9.6370134254944340   F   F   F
  4.0898816265198921  4.3191081760680561  9.6370174916187459   F   F   F
  3.3886823758463138 -0.0998086469148240 11.5001265918296856   T   T   T
  1.5192108689408657  2.3540224100932696 11.5000421695671875   T   T   T
  3.4314584579207215  1.8744095814243806 11.4620763552299696   T   T   T
  1.4764609193359448  4.3282871490525405 11.4621138020827988   T   T   T
  0.8160478825863440  0.0529452224463797 13.2150023488581123   T   T   T
  4.0918098226737536  2.5068188302527821 13.2149774395988953   T   T   T
  1.0353134525200354  1.9387343713919822 13.3913287185330017   T   T   T
  3.8725372513911878  4.3926026554740307 13.3913578719965471   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_2x2/Ni E_tot= -61.57878021 eV
 D3-zero damping= -2.7149961 eV, D3-BJ damping= -3.5104986 eV
Ni
 1.0000000000000000
     4.9077161635400008    0.0000000000000000    0.0000000000000000
     0.0000000000000000    4.9077161635400008    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7797100266724897
  12
```

```
Cartesian
  0.0000000550467280 -0.0000003522015235  8.1594403438688872
  1.2269273019605531  1.2269285729696504  9.8895985175742656
 -0.0000000411793389  0.0000000830949396 11.6200307896094355
 -0.0000000115414995  2.4538580424202157  8.1594468153723874
  1.2269272733274239  3.6807875900381855  9.8895992413638041
 -0.0000001168521267  2.4538581434478592 11.6200377960029382
  2.4538581505405070 -0.0000001899210281  8.1594426392704253
  3.6807888000110771  1.2269285827696597  9.8895988685616008
  2.4538581360818559  0.0000000717800928 11.6200294941275946
  2.4538582255787471  2.4538581581924421  8.1594468707131647
  3.6807887435704689  3.6807874969775978  9.8895989852503519
  2.4538581783592144  2.4538581629442495 11.6200309313869017

Interface: ZnO(11-20)/fcc(100)_2x2/Ir E_tot= -174.29878535 eV
 D3-zero damping= -9.3578689 eV, D3-BJ damping= -9.6126103 eV
Zn  O Zn  O Zn  O Zn  O Ir
 1.0000000000000000
     5.4301264291000013    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4301264291000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.5844023453527321
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.6202203841263558  0.0050783507803370  8.0000000000000000   F   F   F
  1.8101773951661140  2.7201415710766659  8.0000055199296671   F   F   F
  3.6202202803038270  2.0637998113629576  8.0000008619369254   F   F   F
  1.8101780834531387  4.7788630348582144  8.0000049280612373   F   F   F
  0.9051519634740220  0.0050783706452949  9.6370125635575068   F   F   F
  4.5252354036137818  2.7201415909416231  9.6370180834871757   F   F   F
  0.9051518596514924  2.0637998312279153  9.6370134254944340   F   F   F
  4.5252360919008057  4.7788630547231721  9.6370174916187459   F   F   F
  3.8102206292424423  0.0825925171027354 11.3682264945538432   T   T   T
  1.6199850653225505  2.7976344445769827 11.3681924628577562   T   T   T
  3.4688014762982511  2.0246628916553218 11.2167668466778352   T   T   T
  1.9615079143837875  4.7397061161302556 11.2168880369205244   T   T   T
  1.4038630716005311  0.0813110104015173 12.9005126514967365   T   T   T
  4.0262592518511084  2.7962616701919498 12.9005489868197625   T   T   T
  0.5060012936439447  1.8521545532565455 12.7316064061239285   T   T   T
  4.9241058464711598  4.5671658552340526 12.7314874654229673   T   T   T
 -0.0552375261489400 -0.9522897652472535 14.7990019577149337   T   T   T
  1.3457518190889759  0.3743170587228816 16.7065946183974177   T   T   T
 -0.0046882967346027 -0.9758010433236878 18.5571595945335837   T   T   T
  0.0548325059149930  1.7627394075777598 14.7991343242649886   T   T   T
  1.3401099674387467  3.1132879097783333 16.6934330837474860   T   T   T
  0.0043245079399238  1.7392483652079871 18.5571367871493003   T   T   T
  2.6989994013808865 -0.9908830435617493 14.8599995195656103   T   T   T
  4.0896342718672818  0.3981861382255482 16.6934392791644797   T   T   T
  2.7144617882141651 -0.9723594035750502 18.5411828754569612   T   T   T
  2.7308050897491882  1.7242106335901912 14.8600036820088981   T   T   T
  4.0840421552695192  3.0894137776111794 16.7066046603044036   T   T   T
  2.7153213448295048  1.7427344594623753 18.5411180577165275   T   T   T

Oxide reference: ZnO(11-20)/fcc(100)_2x2/Ir E_tot= -69.60240487 eV
 D3-zero damping= -2.1417907 eV, D3-BJ damping= -2.4183095 eV
Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     5.4301264291000013    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4301264291000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.8298334931259674
   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
```

```
  3.6202203841263558  0.0050783507803370  8.0000000000000000   F   F   F
  1.8101773951661140  2.7201415710766659  8.0000055199296689   F   F   F
  3.6202202803038270  2.0637998113629576  8.0000008619369254   F   F   F
  1.8101780834531387  4.7788630348582144  8.0000049280612373   F   F   F
  0.9051519634740220  0.0050783706452949  9.6370125635575086   F   F   F
  4.5252354036137818  2.7201415909416231  9.6370180834871775   F   F   F
  0.9051518596514924  2.0637998312279153  9.6370134254944340   F   F   F
  4.5252360919008057  4.7788630547231721  9.6370174916187459   F   F   F
  3.6103474822111870  0.0496707530714330 11.3365041975721557   T   T   T
  1.8199805140977909  2.7646805609588587 11.3365457985684692   T   T   T
  3.6658848259281127  2.0532733156050815 11.3330227082971025   T   T   T
  1.7644557699598122  4.7683342662505073 11.3330447720167466   T   T   T
  0.7060043089168885  0.2249777819095457 12.7503694977823478   T   T   T
  4.7243070118611667  2.9400445236911676 12.7503896635575629   T   T   T
  0.9712203433545838  2.0705368770564494 12.9803828005963293   T   T   T
  4.4590557029821127  4.7856056777214366 12.9804105077740441   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_2x2/Ir E_tot= -100.5400917 eV
 D3-zero damping= -4.9661077 eV, D3-BJ damping= -5.3821993 eV
Ir
 1.0000000000000000
     5.4301264291000013    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4301264291000013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7797100266724897
  12
Cartesian
 -0.0000000974148793 -0.0000003020706429  8.0392737440039248
  1.3575303755682586  1.3575312161028557  9.8898439758665742
 -0.0000001416227813 -0.0000001254258570 11.7399578814644769
 -0.0000001076612941  2.7150633879145958  8.0392738514600843
  1.3575303460982118  4.0725951158743277  9.8898443162106418
 -0.0000001403400827  2.7150633503208135 11.7399563856684281
  2.7150633461920797 -0.0000002763793306  8.0392745147069444
  4.0725961202411405  1.3575312529105781  9.8898442546383354
  2.7150633846212067 -0.0000001108631846 11.7399566680216569
  2.7150633943600266  2.7150633556237267  8.0392738126711549
  4.0725961120040317  4.0725951074887101  9.8898444098984193
  2.7150633467796315  2.7150633576065077 11.7399572885104551

Interface: ZnO(11-20)/fcc(100)_2x2/Rh E_tot= -156.27166541 eV
 D3-zero damping= -8.2749317 eV, D3-BJ damping= -8.9145159 eV
Zn  O Zn  O Zn  O Zn  O Rh
 1.0000000000000000
     5.3553253905600009    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3553253905600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.5844023453527321
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.5703511503226757  0.0050083955191844  8.0000000000000000   F   F   F
  1.7852418525285734  2.6826710964663563  8.0000055199296671   F   F   F
  3.5703510479303220  2.0353705710415322  8.0000008619369254   F   F   F
  1.7852425313343117  4.7130332751435660  8.0000049280612373   F   F   F
  0.8926833206554055  0.0050084151104986  9.6370125635575068   F   F   F
  4.4628994134213045  2.6826711160576697  9.6370180834871757   F   F   F
  0.8926832182630512  2.0353705906328465  9.6370134254944340   F   F   F
  4.4629000922270414  4.7130332947348803  9.6370174916187459   F   F   F
  3.6821447590228091  0.0365751037004832 11.3676810015867993   T   T   T
  1.6732561639781016  2.7142810583846044 11.3677232682772775   T   T   T
  3.5290512259728333  2.0044189729076862 11.2806192201536444   T   T   T
  1.8262218659848002  4.6821004543575100 11.2807451136637784   T   T   T
  1.1732617561638223  0.0127735335081560 12.9694392690647309   T   T   T
  4.1819518688434600  2.6902652600061256 12.9694177426897568   T   T   T
```

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  0.7932063370179686  1.9579739022737288 12.9652770440770446   T   T   T
  4.5611486725608978  4.6356863568269686 12.9660001192526320   T   T   T
 -0.0399564745368588 -0.8070688324516730 15.0216869372014905   T   T   T
  1.3447268145738438  0.5127219827278103 16.8662524525676574   T   T   T
 -0.0094450615259383 -0.8110368840467915 18.6846470025291822   T   T   T
  0.0401885665410342  1.8705066711776477 15.0217865640679094   T   T   T
  1.3445044138919000  3.2269064350269216 16.8454369911252009   T   T   T
  0.0102496306413238  1.8668342342917152 18.6850022570842960   T   T   T
  2.6539999661239659 -0.8025893454679333 14.9684580934295379   T   T   T
  4.0113084451111298  0.5491283801829618 16.8455836829256143   T   T   T
  2.6779768429051178 -0.8134291439605773 18.6973210543935267   T   T   T
  2.7016322359902341  1.8751807813229258 14.9688459748907352   T   T   T
  4.0111283695100424  3.1903124966793572 16.8663449932950940   T   T   T
  2.6780076803166200  1.8640530349702389 18.6970637184275681   T   T   T

Oxide reference: ZnO(11-20)/fcc(100)_2x2/Rh E_tot= -69.58074035 eV
 D3-zero damping= -2.1759579 eV, D3-BJ damping= -2.4728843 eV
Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     5.3553253905600009    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3553253905600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.8298334931259674
   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.5703511503226757  0.0050083955191844  8.0000000000000000   F   F   F
  1.7852418525285734  2.6826710964663563  8.0000055199296689   F   F   F
  3.5703510479303220  2.0353705710415322  8.0000008619369254   F   F   F
  1.7852425313343117  4.7130332751435660  8.0000049280612373   F   F   F
  0.8926833206554055  0.0050084151104986  9.6370125635575086   F   F   F
  4.4628994134213045  2.6826711160576697  9.6370180834871775   F   F   F
  0.8926832182630512  2.0353705906328465  9.6370134254944340   F   F   F
  4.4629000922270414  4.7130332947348803  9.6370174916187459   F   F   F
  3.5761766927898524  0.0333476161307955 11.3540651220543207   T   T   T
  1.7792942640821450  2.7110261993739471 11.3540913035270776   T   T   T
  3.6307556910847123  2.0275025425398701 11.3454648904961370   T   T   T
  1.7247045385362270  4.7051777285517380 11.3455219865580776   T   T   T
  0.7090299316323700  0.2081872769208255 12.8049663039355899   T   T   T
  4.6463850922863106  2.8858589834777346 12.8049062447365287   T   T   T
  0.9870787540407904  2.0524413998253990 13.0388912487933677   T   T   T
  4.3683278061997424  4.7301019572675544 13.0389002760709314   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_2x2/Rh E_tot= -82.84737428 eV
 D3-zero damping= -4.0067948 eV, D3-BJ damping= -4.8322246 eV
Rh
 1.0000000000000000
     5.3553253905600009    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3553253905600009    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7797100266724897
  12
Cartesian
  0.0000000675551330 -0.0000001478533706  8.0461948549860978
  1.3388300455008844  1.3388309609681610  9.8897383766557230
  0.0000000929274772  0.0000002434868388 11.7331398522598480
  0.0000000922819710  2.6776625862883296  8.0461977719998625
  1.3388300211861375  4.0164943591445148  9.8897389504958451
  0.0000001120882429  2.6776625810519290 11.7331418005315431
  2.6776626391219924 -0.0000001038800543  8.0461964319829278
  4.0164953448155662  1.3388309494752662  9.8897387455005124
  2.6776626084432298  0.0000002119684273 11.7331380995218559
  2.6776626304658770  2.6776626373434769  8.0461979839043121
  4.0164953547913056  4.0164942947694922  9.8897389485603426
  2.6776625749966536  2.6776625880408882 11.7331393623318103
```

```
Interface: ZnO(11-20)/fcc(100)_2x2/Os E_tot= -197.502203 eV
 D3-zero damping= -7.7273775 eV, D3-BJ damping= -8.7473273 eV
Zn  O Zn  O Zn  O Zn  O Os
 1.0000000000000000
     5.4168285661600013    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4168285661600013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.5844023453527321
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.6113548088751579  0.0050659143824888  8.0000000000000000   F   F   F
  1.8057444429665102  2.7134802031947456  8.0000055199296671   F   F   F
  3.6113547053068804  2.0587457619986500  8.0000008619369254   F   F   F
  1.8057451295679856  4.7671600540020007  8.0000049280612373   F   F   F
  0.9029353324420730  0.0050659341987994  9.6370125635575068   F   F   F
  4.5141535326934275  2.7134802230110555  9.6370180834871757   F   F   F
  0.9029352288737948  2.0587457818149604  9.6370134254944340   F   F   F
  4.5141542192949018  4.7671600738183111  9.6370174916187459   F   F   F
  3.7657175544610886  0.0640191729521295 11.3543865980226180   T   T   T
  1.6511397529553951  2.7723521053303251 11.3544611315547890   T   T   T
  3.5134742217827020  2.0281475835760601 11.2416730148108019   T   T   T
  1.9034332412835375  4.7364739487986878 11.2417401558299570   T   T   T
  1.3777613298782780  0.0574827740894238 12.9566315710774429   T   T   T
  4.0390603442511690  2.7659054667631193 12.9566054141108111   T   T   T
  0.6236032160290084  1.9233373505207616 12.8732799161908229   T   T   T
  4.7931719608573280  4.6318529708898133 12.8732318155924261   T   T   T
 -0.0824999484580021 -0.9067620530446000 14.8964679958140422   T   T   T
  1.3218387529558278  0.3757410908981718 16.7797389687017322   T   T   T
 -0.0092967556391432 -0.9537974628869494 18.6509725420282884   T   T   T
  0.0821416889990042  1.8016298580792696 14.8965383965975615   T   T   T
  1.3302790035659910  3.1869927700949403 16.7460278373122478   T   T   T
  0.0089507955415713  1.7546918064497068 18.6508909168932924   T   T   T
  2.6930212719419515 -0.9491399264038664 14.9503930474683600   T   T   T
  4.0859717622634344  0.4785730354621354 16.7460217142009675   T   T   T
  2.7073327458492473 -0.9442405765846245 18.6347394892830920   T   T   T
  2.7233994527600403  1.7593836453452480 14.9503433747687371   T   T   T
  4.0946128937846380  3.0840796713144547 16.7796726243012095   T   T   T
  2.7092674424190233  1.7642200362431806 18.6347052424551478   T   T   T

Oxide reference: ZnO(11-20)/fcc(100)_2x2/Os E_tot= -69.60678297 eV
 D3-zero damping= -2.1475307 eV, D3-BJ damping= -2.4277117 eV
Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     5.4168285661600013    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4168285661600013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.8298334931259674
   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.6113548088751579  0.0050659143824888  8.0000000000000000   F   F   F
  1.8057444429665102  2.7134802031947456  8.0000055199296689   F   F   F
  3.6113547053068804  2.0587457619986500  8.0000008619369254   F   F   F
  1.8057451295679856  4.7671600540020007  8.0000049280612373   F   F   F
  0.9029353324420730  0.0050659341987994  9.6370125635575086   F   F   F
  4.5141535326934275  2.7134802230110555  9.6370180834871775   F   F   F
  0.9029352288737948  2.0587457818149604  9.6370134254944340   F   F   F
  4.5141542192949018  4.7671600738183111  9.6370174916187459   F   F   F
  3.6037319840845368  0.0473572900229910 11.3390270004406766   T   T   T
  1.8132450542133312  2.7557999702862941 11.3390137216396418   T   T   T
  3.6599313369023876  2.0489560117899375 11.3355833930014782   T   T   T
  1.7571062273852409  4.7573913535574626 11.3356283302073262   T   T   T
  0.7068749925081534  0.2229769432654510 12.7611787368178096   T   T   T
```

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  4.7101312485510203  2.9313691793987369 12.7611539770075435   T   T   T
  0.9739677279394698  2.0683271381754751 12.9907797193142880   T   T   T
  4.4430218341235150  4.7767245614235394 12.9908152394960137   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_2x2/Os E_tot= -123.42130289 eV
 D3-zero damping= -3.8571648 eV, D3-BJ damping= -4.6225372 eV
Os
 1.0000000000000000
     5.4168285661600013    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.4168285661600013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7797100266724897
  12
Cartesian
  0.0000009170170050  0.0000009000254444  8.0400349104926825
  1.3542066610327157  1.3542071992517315  9.8896860622116520
  0.0000010168515597  0.0000012799037434 11.7393524934856330
  0.0000009759942430  2.7084130838900733  8.0400365819814503
  1.3542069449180745  4.0626213258514268  9.8896867621530351
  0.0000009618138197  2.7084131023682581 11.7393546451326571
  2.7084133994067794  0.0000011102051700  8.0400353588850333
  4.0626217889180838  1.3542070310956245  9.8896864396291218
  2.7084133807828912  0.0000013157156153 11.7393519130132731
  2.7084134795194754  2.7084131190609777  8.0400371746037802
  4.0626214669566503  4.0626216202767980  9.8896865338012212
  2.7084133274266287  2.7084128768573277 11.7393523599119707

Interface: ZnO(11-20)/fcc(100)_2x2/Ru E_tot= -176.71630792 eV
 D3-zero damping= -8.1261698 eV, D3-BJ damping= -8.7402305 eV
Zn  O Zn  O Zn  O Zn  O Ru
 1.0000000000000000
     5.3323894838800010    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3323894838800010    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.5844023453527321
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.5550599710148822  0.0049869454514729  8.0000000000000000   F   F   F
  1.7775959790204945  2.6711816930343733  8.0000055199296671   F   F   F
  3.5550598690610573  2.0266534406951826  8.0000008619369254   F   F   F
  1.7775966549190285  4.6928481914194338  8.0000049280612373   F   F   F
  0.8888601166772802  0.0049869649588810  9.6370125635575068   F   F   F
  4.4437856085628935  2.6711817125417809  9.6370180834871757   F   F   F
  0.8888600147234540  2.0266534602025907  9.6370134254944340   F   F   F
  4.4437862844614262  4.6928482109268419  9.6370174916187459   F   F   F
  3.6450796738979370 -0.0095357855349076 11.3699935287304257   T   T   T
  1.6875514856467591  2.6564967545494622 11.3700084186680925   T   T   T
  3.5782100509662560  1.9762265526366096 11.2893706106146681   T   T   T
  1.7545926273424979  4.6422906884078987 11.2893554304933055   T   T   T
  1.2130257138507168 -0.0701911408870090 13.0275830051184993   T   T   T
  4.1190906685245015  2.5963674666287577 13.0279044204977215   T   T   T
  1.1495868480792724  1.9535420908074552 13.1763075429981313   T   T   T
  4.1838158892883337  4.6200636699435291 13.1759367912297236   T   T   T
 -0.0432422584727218 -0.7905656757178222 15.0358477929113530   T   T   T
  1.3521488120468896  0.4562081360552594 16.8156512739333976   T   T   T
 -0.0321015562071660 -0.7941975820348771 18.6454303012347502   T   T   T
  0.0432744544553182  1.8754184001639933 15.0358975586357158   T   T   T
  1.3596285924088474  3.2906442610295472 16.7724876270779824   T   T   T
  0.0322278802087062  1.8720185745584164 18.6452632479954659   T   T   T
  2.7544884531291287 -0.7781598448472288 14.9401260276231227   T   T   T
  3.9729085164984665  0.6241549058000544 16.7729687096934157   T   T   T
  2.6318792825063073 -0.8164856202853936 18.6807802962383356   T   T   T
  2.5778983057230520  1.8878295975055333 14.9401167099854781   T   T   T
  3.9797968576102791  3.1223122439839002 16.8153805021588170   T   T   T
```

```
  2.7008320367787073  1.8497398468577166 18.6808571635188407   T   T   T

Oxide reference: ZnO(11-20)/fcc(100)_2x2/Ru E_tot= -69.55151916 eV
 D3-zero damping= -2.186859 eV, D3-BJ damping= -2.4880247 eV
Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
     5.3323894838800010    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3323894838800010    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.8298334931259674
   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.5550599710148822  0.0049869454514729  8.0000000000000000   F   F   F
  1.7775959790204945  2.6711816930343733  8.0000055199296689   F   F   F
  3.5550598690610573  2.0266534406951826  8.0000008619369254   F   F   F
  1.7775966549190285  4.6928481914194338  8.0000049280612373   F   F   F
  0.8888601166772802  0.0049869649588810  9.6370125635575086   F   F   F
  4.4437856085628935  2.6711817125417809  9.6370180834871775   F   F   F
  0.8888600147234540  2.0266534602025907  9.6370134254944340   F   F   F
  4.4437862844614262  4.6928482109268419  9.6370174916187459   F   F   F
  3.5665804037457285  0.0231957271184885 11.3612810321794964   T   T   T
  1.7663300550888521  2.6893949129263377 11.3611315519328304   T   T   T
  3.6206453288369564  2.0150712671548225 11.3514431543718377   T   T   T
  1.7123134202852457  4.6812823701499857 11.3513519997540886   T   T   T
  0.7159272248102132  0.1931054176787050 12.8318533374883685   T   T   T
  4.6170573071376486  2.8592816752881025 12.8319192786160965   T   T   T
  0.9894662488372453  2.0397796779869970 13.0583530328249058   T   T   T
  4.3435693980938046  4.7059229578715662 13.0584210287197209   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_2x2/Ru E_tot= -102.47064909 eV
 D3-zero damping= -3.7832709 eV, D3-BJ damping= -4.615082 eV
Ru
 1.0000000000000000
     5.3323894838800010    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.3323894838800010    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7797100266724897
  12
Cartesian
  0.0000013138136513  0.0000007620727823  8.0555312907339669
  1.3330981937635482  1.3330975817961219  9.8894541927752950
  0.0000018392597490  0.0000027726182664 11.7240856372190247
  0.0000012593270667  2.6661924900189877  8.0555420923333028
  1.3330974974474927  3.9992916724094982  9.8894579326752972
  0.0000016359158353  2.6661924834135005 11.7240959094859001
  2.6661928785976992  0.0000015373814790  8.0555267229222363
  3.9992923028669773  1.3330976681365583  9.8894533246018970
  2.6661938984805422  0.0000027501707430 11.7240753464264156
  2.6661930461169105  2.6661926180958901  8.0555367259275688
  3.9992907802073705  3.9992929318302117  9.8894561007406878
  2.6661934041310831  2.6661924303288749 11.7240859640680775

Interface: O-a-SiO2(0001)/fcc(111)_sqrt13/Au E_tot= -976.78286939 eV
 D3-zero damping= -28.4805532 eV, D3-BJ damping= -31.6119659 eV
Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O
Si  O  H Au
 1.0000000000000000
    10.4515979269385308    0.0000000000000000    0.0000000000000000
    -5.2257989634692628    9.0513493148695439    0.0000000000000000
     0.0000000000000023    0.0000000000000040   37.2517640797182210
   2   5   3   6   3   7   2   2   5   3   6   3   7   2   2   5   3   6
3   7   2   2   5   3   6   3   7   2  39
Selective dynamics
Cartesian
```

2.6947900201070278	0.1933043429058221	9.0169746245084816	F	F	F
-1.3121456715960300	2.4964361649897735	10.8612336967246357	F	F	F
2.4173342951357704	2.7586919526168669	11.6081185941916658	F	F	F
3.6677137190527764	1.4862905002695610	9.5654178022134708	F	F	F
-0.6602915834112228	3.9592057746683058	10.2987723773365900	F	F	F
1.1628214790510143	3.6155877692007312	8.2518078419286880	F	F	F
-0.2053574456059191	1.8086006664657244	11.9218080039603862	F	F	F
2.7453567882958225	-0.0472036976283530	14.5050718430130097	F	F	F
1.2859327537291589	2.1170312127402315	12.6701466762358947	F	F	F
-1.2514421566085185	2.3087333411297539	16.2701552737491930	T	T	T
2.6451552153090048	2.4711458986926389	17.1188779653142937	T	T	T
3.7029043940863264	1.0821753596037191	15.1653689645917034	T	T	T
1.8285117866822465	0.6328231310567688	13.2917821082657603	F	F	F
-0.8703031799012471	3.7206149800439392	15.5401580921708415	T	T	T
1.1133261514530117	3.2377480865045731	13.8903255655927040	F	F	F
0.0011906650450867	1.8558890495226343	17.2140963652319954	T	T	T
0.0384259642926433	4.4183125423424627	19.7652704429103849	T	T	T
1.3569153221500823	2.1884784368263990	18.0672027124385437	T	T	T
4.3617477639227591	2.0799567234224394	21.5532383144795254	T	T	T
3.8520262987176794	0.9922793805199306	20.4571653271680027	T	T	T
1.6528700761663231	0.8895904309810084	19.0149733844605038	T	T	T
-0.9203411498499041	3.2981720286158072	20.4552408452155454	T	T	T
1.1343298112997346	3.5816397420473134	18.8939285829802444	T	T	T
0.3235300536903858	1.7013233752441577	22.2919462261302073	T	T	T
3.1604090443609509	2.1051241573972730	22.7083849833279601	T	T	T
1.4504788782990996	0.7163636327050370	8.0000000000000000	F	F	F
1.2389464268462906	1.7396828418631378	8.0158744918591083	F	F	F
2.0781711762066011	4.0422552258167554	8.0308754104330902	F	F	F
0.0818905383723960	4.7189790003405951	9.0169746245084816	F	F	F
-3.9250451533306614	7.0221108224245468	10.8612336967246357	F	F	F
-0.1955651865988614	7.2843666100516407	11.6081185941916658	F	F	F
1.0548142373181446	6.0119651577043332	9.5654178022134708	F	F	F
-3.2731910651458542	8.4848804321030773	10.2987723773365900	F	F	F
-1.4500780026836173	8.1412624266355031	8.2518078419286880	F	F	F
-2.8182569273405509	6.3342753239004965	11.9218080039603862	F	F	F
0.1324573065611909	4.4784709598064190	14.5050718430130097	F	F	F
-1.3269667280054724	6.6427058701750044	12.6701466762358947	F	F	F
-3.8953737760797238	6.8310717724058678	16.2533512327572822	T	T	T
-0.0530235628975917	7.1159871548086722	17.0672364817365292	T	T	T
1.0660720269555908	5.6109032034847743	15.2044759429488572	T	T	T
-0.7843876950523851	5.1584977884915419	13.2917821082657603	F	F	F
-3.4955155076795887	8.2634949930117312	15.5584005576381710	T	T	T
-1.4995733302816199	7.7634227439393459	13.8903255655927040	F	F	F
-2.6323019773167333	6.3077038733953898	17.1316778545258614	T	T	T
-2.4941331564401725	9.0322687986968582	19.8511494165371793	T	T	T
-1.3159714620556984	6.6972119873696068	18.0019574606114716	T	T	T
1.0532364499480542	6.8145838041493176	21.5481805325773195	T	T	T
0.8263347201292218	5.3523014768913235	20.8419109224776662	T	T	T
-0.9107624086437558	5.3790414032425593	18.8617777864370844	T	T	T
-3.3002621842367428	8.1631625831652812	20.9737522602213389	T	T	T
-1.6829574430042760	7.9905326164975872	18.9064881377608600	T	T	T
-2.8672422948232725	5.9910608968732300	22.5781198467439843	T	T	T
-0.3088412042224180	7.3622109771898430	22.2534030229395583	T	T	T
-1.1624206034355320	5.2420382901398099	8.0000000000000000	F	F	F
-1.3739530548883410	6.2653574992979104	8.0158744918591083	F	F	F
-0.5347283055280305	8.5679298832515283	8.0308754104330902	F	F	F
7.9205889835762937	0.1933043429058221	9.0169746245084816	F	F	F
3.9136532918732359	2.4964361649897735	10.8612336967246357	F	F	F
7.6431332586050358	2.7586919526168669	11.6081185941916658	F	F	F
8.8935126825220419	1.4862905002695610	9.5654178022134708	F	F	F
4.5655073800580430	3.9592057746683058	10.2987723773365900	F	F	F
6.3886204425202804	3.6155877692007312	8.2518078419286880	F	F	F
5.0204415178633468	1.8086006664657244	11.9218080039603862	F	F	F

7.9711557517650888	-0.0472036976283530	14.5050718430130097	F	F	F
6.5117317171984244	2.1170312127402315	12.6701466762358947	F	F	F
3.9948214922530481	2.2792310032942802	16.2439471037429541	T	T	T
7.8458332383088534	2.6197589865142534	17.1067147447511410	T	T	T
8.9000720594191272	1.0748460410818770	15.2280886130053119	T	T	T
7.0543107501515125	0.6328231310567688	13.2917821082657603	F	F	F
4.3523157236789691	3.7210465912786330	15.5506641775846237	T	T	T
6.3391251149222780	3.2377480865045731	13.8903255655927040	F	F	F
5.2679498597616847	1.8114395567539092	17.1468800994366184	T	T	T
5.2271183553409202	4.5346881909578514	19.8007016409020871	T	T	T
6.5682746245906634	2.2384598078058255	18.0354304659306912	T	T	T
9.3490247745901041	2.1635752838056899	21.6073112328993062	T	T	T
8.6502077337395455	0.8163641010602388	20.9932833613784808	T	T	T
6.9887423363656200	0.9622014460831829	18.9448180427932300	T	T	T
4.4561516673632502	3.5906106823557233	20.8947151614827291	T	T	T
6.1768859578116677	3.5640411616682530	18.9002431080839841	T	T	T
5.7940674818798152	1.6832807460999817	22.2285173991837084	T	T	T
8.4158570935733046	2.9281834318945306	22.7536032764154719	T	T	T
6.6762778417683650	0.7163636327050370	8.0000000000000000	F	F	F
6.4647453903155565	1.7396828418631378	8.0158744918591083	F	F	F
7.3039701396758669	4.0422552258167554	8.0308754104330902	F	F	F
5.3076895018416623	4.7189790003405951	9.0169746245084816	F	F	F
1.3007538101386042	7.0221108224245468	10.8612336967246357	F	F	F
5.0302337768704044	7.2843666100516407	11.6081185941916658	F	F	F
6.2806132007874114	6.0119651577043332	9.5654178022134708	F	F	F
1.9526078983234114	8.4848804321030773	10.2987723773365900	F	F	F
3.7757209607856486	8.1412624266355031	8.2518078419286880	F	F	F
2.4075420361287154	6.3342753239004965	11.9218080039603862	F	F	F
5.3582562700304566	4.4784709598064190	14.5050718430130097	F	F	F
3.8988322354637934	6.6427058701750044	12.6701466762358947	F	F	F
1.3182161474534688	6.8581731294079322	16.2410756172612665	T	T	T
5.2189399422804446	7.0533379057896495	17.1511327485300100	T	T	T
6.2651737126584379	5.6395419158194011	15.1712452049581650	T	T	T
4.4414112684168803	5.1584977884915419	13.2917821082657603	F	F	F
1.6961575503017103	8.2672542337920749	15.5093792751483495	T	T	T
3.7262256331876458	7.7634227439393459	13.8903255655927040	F	F	F
2.5675469724886866	6.4641161611322220	17.2006336338139860	T	T	T
2.6315780872314747	8.9925095399066564	19.8644651568903967	T	T	T
3.9083529113251165	6.7520257781579991	18.0773129437857207	T	T	T
6.5312504134891753	6.7872872711288394	21.6062602445129599	T	T	T
6.1594113275112683	5.6935723700037535	20.4610149014754406	T	T	T
4.1308433129006445	5.3656127261245121	18.9192948831535297	T	T	T
1.5843480603547178	7.9270097250042202	20.4964091274575679	T	T	T
3.6976297429358382	8.0962498655783151	18.9942778588153196	T	T	T
2.2773426953309084	6.5528206566595975	22.6515728010506834	T	T	T
5.1665345112360050	7.2371256011282137	22.4562307809370836	T	T	T
4.0633783600337336	5.2420382901398099	8.0000000000000000	F	F	F
3.8518459085809251	6.2653574992979104	8.0158744918591083	F	F	F
4.6910706579412356	8.5679298832515283	8.0308754104330902	F	F	F
0.1533990693853499	-0.2378448283625430	24.0501712884123009	T	T	T
2.9146378117132179	0.3588414547228355	24.1941912084110484	T	T	T
8.4216508095191944	1.6662928398519474	24.4982594630238175	T	T	T
0.8228370780951295	2.5180502075867568	24.1938379483248056	T	T	T
3.7851190911155155	3.3099726657300352	24.3614633070743203	T	T	T
-1.1116917586457515	4.5785182865050871	24.2637097861275919	T	T	T
1.6911399654917443	5.1512810001739417	24.2226982565841595	T	T	T
4.6254833807447699	5.9289220680439048	24.1805624155276853	T	T	T
-0.2643668444170934	7.3125926729278721	24.3237978244065971	T	T	T
2.5988384564769054	8.0484954007871288	24.2611705680507015	T	T	T
8.2183027805758488	0.2860667339550741	26.7681235161384166	T	T	T
0.5459950598427527	1.0319587839767053	26.5867353567009985	T	T	T
6.1948282296284569	2.4319816582850313	26.7119018525209313	T	T	T
-1.4271941142828402	3.1805395486542523	26.7848065160244388	T	T	T

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  1.3760778155335938  3.7952237974501517 26.6036148113320117   T   T   T
 -0.6108846710871942  5.9520046685176276 26.7206347232346779   T   T   T
  2.1920202008003145  6.6084356695540576 26.6924584294423113   T   T   T
  0.1819263131049028  8.7464464917830682 26.6784191838531335   T   T   T
 -5.0344224645690412  8.7176457085694175 29.1768710417617640   T   T   T
 -1.8295443168910461  1.7358796388004771 29.2283768463869045   T   T   T
  0.9821215470976745  2.4361464544763876 29.1182042975850806   T   T   T
  6.6159711073066134  3.8093707991983727 29.2776321337962990   T   T   T
 -1.0231184898805095  4.5610005809915757 29.2554259591120704   T   T   T
  1.7871175303758260  5.1944826607752308 29.1439771192165900   T   T   T
 -3.0200240467390986  6.6419765767743844 29.2759207981028915   T   T   T
 -0.1993640334809820  7.3371314008572686 29.2093654886252168   T   T   T
  2.6055207830160905  8.0046898749362061 29.2338748802401476   T   T   T
  5.8028386181084111  1.0484062615050140 29.2378532023381155   T   T   T
  5.6933251100163060  1.0238694443469023 24.2274390927699876   T   T   T
  6.5552017650405299  3.8965044237453172 24.3023793771158871   T   T   T
 -3.0302165932381611  6.7174435244263515 24.5310033987016034   T   T   T
 -2.6283017058865594  8.0798883865784870 26.7988965065194087   T   T   T
  3.3792992630019825  1.7434007379248118 26.6983277960796279   T   T   T
  4.2184749362739300  4.5994201775319361 26.6760533744886743   T   T   T
 -3.4276272542786606  5.2009361691429037 26.8341101829994813   T   T   T
  5.0499611190243572  7.3467433269394267 26.6048102032373137   T   T   T
  2.9987843419507296  0.3760141296991489 29.2752405480490516   T   T   T
  3.8099297341564236  3.1570675106678059 29.1656824169711619   T   T   T
  4.6230638202859131  5.9372773497705724 29.1489545431015422   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Au E_tot= -879.84818587 eV
 D3-zero damping= -8.0679724 eV, D3-BJ damping= -11.5446783 eV
Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H
O  H Si  O Si  O Si  O  H  O  H
 1.0000000000000000
    10.4515979269385308    0.0000000000000000    0.0000000000000000
    -5.2257989634692628    9.0513493148695439    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.6897910220632006
   2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.6947900201070278  0.1933043429058221  9.0169746245084816   F   F   F
 -1.3121456715960300  2.4964361649897735 10.8612336967246357   F   F   F
  2.4173342951357704  2.7586919526168669 11.6081185941916623   F   F   F
  3.6677137190527764  1.4862905002695610  9.5654178022134708   F   F   F
 -0.6602915834112228  3.9592057746683058 10.2987723773365900   F   F   F
  1.1628214790510143  3.6155877692007312  8.2518078419286844   F   F   F
 -0.2053574456059191  1.8086006664657244 11.9218080039603862   F   F   F
  2.7453567882958225 -0.0472036976283530 14.5050718430130097   F   F   F
  1.2859327537291589  2.1170312127402315 12.6701466762358947   F   F   F
 -1.2686294361411021  2.3072346513776831 16.2533016931944729   T   T   T
  2.6014713573602322  2.5513355172245369 17.1128222494477598   T   T   T
  3.6768295342515009  1.0866203662448641 15.1981602817107433   T   T   T
  1.8285117866822465  0.6328231310567688 13.2917821082657603   F   F   F
 -0.8846715829732642  3.7305446299962441 15.5443240228137984   T   T   T
  1.1133261514530117  3.2377480865045731 13.8903255655927005   F   F   F
 -0.0145098688064409  1.8440306104160216 17.1833381547193156   T   T   T
  0.1049955308743352  4.5293973135153136 19.8318744311870212   T   T   T
  1.3211224133741153  2.1882436873104436 18.0484566662507326   T   T   T
  4.0537686171989034  2.2592576918042093 21.6434689562550631   T   T   T
  3.6797547015568393  1.0818399647229409 20.5758818038279259   T   T   T
  1.6607026858709772  0.8503599742696062 18.9200584311604487   T   T   T
 -0.7218226787440293  3.6473702775934025 20.9161633250138408   T   T   T
  1.0305018692191701  3.5127157548095798 18.9566407796215834   T   T   T
  0.1682766318411443  1.7327268894005736 22.4707722012749613   T   T   T
  2.8211886256520322  2.6591238259582775 22.6280392441391349   T   T   T
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1.9068367241464554	2.2947963830085083	22.5387469818415092	T	T	T
0.1641306712396358	0.7798822517012876	22.6897938363489118	T	T	T
1.4504788782990996	0.7163636327050370	8.0000000000000000	F	F	F
1.2389464268462906	1.7396828418631378	8.0158744918591047	F	F	F
2.0781711762066011	4.0422552258167554	8.0308754104330866	F	F	F
0.0818905383723965	4.7189790003405943	9.0169746245084816	F	F	F
-3.9250451533306614	7.0221108224245459	10.8612336967246357	F	F	F
-0.1955651865988610	7.2843666100516389	11.6081185941916623	F	F	F
1.0548142373181451	6.0119651577043332	9.5654178022134708	F	F	F
-3.2731910651458542	8.4848804321030773	10.2987723773365900	F	F	F
-1.4500780026836171	8.1412624266355031	8.2518078419286844	F	F	F
-2.8182569273405504	6.3342753239004965	11.9218080039603862	F	F	F
0.1324573065611911	4.4784709598064190	14.5050718430130097	F	F	F
-1.3269667280054724	6.6427058701750035	12.6701466762358947	F	F	F
-3.8815289178757331	6.8329093088124555	16.2533016931944729	T	T	T
-0.0114281243743993	7.0770101746593088	17.1128222494477598	T	T	T
1.0639300525168698	5.6122950236796365	15.1981602817107433	T	T	T
-0.7843876950523849	5.1584977884915411	13.2917821082657603	F	F	F
-3.4975710647078957	8.2562192874310156	15.5443240228137984	T	T	T
-1.4995733302816197	7.7634227439393451	13.8903255655927005	F	F	F
-2.6274093505410723	6.3697052678507937	17.1833381547193156	T	T	T
-2.5079039508602965	9.0550719709500846	19.8318744311870212	T	T	T
-1.2917770683605161	6.7139183447452151	18.0484566662507326	T	T	T
1.4408691354642724	6.7849323492389813	21.6434689562550631	T	T	T
1.0668552198222079	5.6075146221577130	20.5758818038279259	T	T	T
-0.9521967958636542	5.3760346317043775	18.9200584311604487	T	T	T
-3.3347221604786608	8.1730449350281749	20.9161633250138408	T	T	T
-1.5823976125154613	8.0383904122443521	18.9566407796215834	T	T	T
-2.4446228498934870	6.2584015468353451	22.4707722012749613	T	T	T
0.2082891439174009	7.1847984833930489	22.6280392441391349	T	T	T
-0.7060627575881758	6.8204710404432802	22.5387469818415092	T	T	T
-2.4487688104949954	5.3055569091360590	22.6897938363489118	T	T	T
-1.1624206034355318	5.2420382901398090	8.0000000000000000	F	F	F
-1.3739530548883407	6.2653574992979095	8.0158744918591047	F	F	F
-0.5347283055280303	8.5679298832515265	8.0308754104330866	F	F	F
7.9205889835762928	0.1933043429058221	9.0169746245084816	F	F	F
3.9136532918732354	2.4964361649897735	10.8612336967246357	F	F	F
7.6431332586050358	2.7586919526168669	11.6081185941916623	F	F	F
8.8935126825220419	1.4862905002695610	9.5654178022134708	F	F	F
4.5655073800580421	3.9592057746683058	10.2987723773365900	F	F	F
6.3886204425202795	3.6155877692007312	8.2518078419286844	F	F	F
5.0204415178633459	1.8086006664657244	11.9218080039603862	F	F	F
7.9711557517650879	-0.0472036976283530	14.5050718430130097	F	F	F
6.5117317171984244	2.1170312127402315	12.6701466762358947	F	F	F
3.9571695273281637	2.3072346513776831	16.2533016931944729	T	T	T
7.8272703208294976	2.5513355172245369	17.1128222494477598	T	T	T
8.9026284977207677	1.0866203662448641	15.1981602817107433	T	T	T
7.0543107501515117	0.6328231310567688	13.2917821082657603	F	F	F
4.3411273804960011	3.7305446299962441	15.5443240228137984	T	T	T
6.3391251149222771	3.2377480865045731	13.8903255655927005	F	F	F
5.2112891089485389	1.8440306104160216	17.1833381547193156	T	T	T
5.3307944943436008	4.5293973135153136	19.8318744311870212	T	T	T
6.5469213768433807	2.1882436873104436	18.0484566662507326	T	T	T
9.2795675806681679	2.2592576918042093	21.6434689562550631	T	T	T
8.9055536650261047	1.0818399647229409	20.5758818038279259	T	T	T
6.8865016493402429	0.8503599742696062	18.9200584311604487	T	T	T
4.5039762847252360	3.6473702775934025	20.9161633250138408	T	T	T
6.2563008469741490	3.5127157548095798	18.9566407796215834	T	T	T
5.3940755953104098	1.7327268894005736	22.4707722012749613	T	T	T
8.0469875891212990	2.6591238259582775	22.6280392298534210	T	T	T
7.1326356876157213	2.2947963830085083	22.5387469818415092	T	T	T
5.3899296347089010	0.7798822517012876	22.6897938363489118	T	T	T
6.6762778417683650	0.7163636327050370	8.0000000000000000	F	F	F

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  6.4647453903155565  1.7396828418631378  8.0158744918591047   F   F   F
  7.3039701396758669  4.0422552258167554  8.0308754104330866   F   F   F
  5.3076895018416614  4.7189790003405943  9.0169746245084816   F   F   F
  1.3007538101386040  7.0221108224245459 10.8612336967246357   F   F   F
  5.0302337768704044  7.2843666100516389 11.6081185941916623   F   F   F
  6.2806132007874105  6.0119651577043332  9.5654178022134708   F   F   F
  1.9526078983234112  8.4848804321030773 10.2987723773365900   F   F   F
  3.7757209607856481  8.1412624266355031  8.2518078419286844   F   F   F
  2.4075420361287150  6.3342753239004965 11.9218080039603862   F   F   F
  5.3582562700304566  4.4784709598064190 14.5050718430130097   F   F   F
  3.8988322354637930  6.6427058701750035 12.6701466762358947   F   F   F
  1.3442700455935319  6.8329093088124555 16.2533016931944729   T   T   T
  5.2143708390948662  7.0770101746593088 17.1128222494477598   T   T   T
  6.2897290159861354  5.6122950236796365 15.1981602817107433   T   T   T
  4.4414112684168803  5.1584977884915411 13.2917821082657603   F   F   F
  1.7282278987613697  8.2562192874310156 15.5443240228137984   T   T   T
  3.7262256331876458  7.7634227439393451 13.8903255655927005   F   F   F
  2.5983896129281931  6.3697052678507937 17.1833381547193156   T   T   T
  2.7178950126089689  9.0550719709500846 19.8318744311870212   T   T   T
  3.9340218951087493  6.7139183447452151 18.0484566662507326   T   T   T
  6.6666680989335374  6.7849323492389813 21.6434689562550631   T   T   T
  6.2926541832914733  5.6075146221577130 20.5758818038279259   T   T   T
  4.2736021676056115  5.3760346317043775 18.9200584311604487   T   T   T
  1.8910768029906049  8.1730449350281749 20.9161633250138408   T   T   T
  3.6434013652395185  8.0383904122443521 18.9566407796215834   T   T   T
  2.7811761135757784  6.2584015468353451 22.4707722012749613   T   T   T
  5.4340881073866667  7.1847984833930489 22.6280392441391349   T   T   T
  4.5197362058810899  6.8204710404432802 22.5387469818415092   T   T   T
  2.7770301529742700  5.3055569091360590 22.6897938363489118   T   T   T
  4.0633783600337336  5.2420382901398090  8.0000000000000000   F   F   F
  3.8518459085809247  6.2653574992979095  8.0158744918591047   F   F   F
  4.6910706579412356  8.5679298832515265  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Au E_tot= -134.45156351 eV
 D3-zero damping= -16.876087 eV, D3-BJ damping= -17.2990027 eV
Au
 1.0000000000000000
    10.4515979269385308    0.0000000000000000    0.0000000000000000
    -5.2257989634692628    9.0513493148695439    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000676436712382  0.0000262980167339  7.8595086384984993
  2.8138849800795245  0.6978029952216056  7.8587478611780330
  8.4404065115875273  2.0880242030657707  7.8588050378192467
  0.8030089517970711  2.7856375619618721  7.8587901869474672
  3.6184955259381160  3.4808666731628848  7.8571738965841966
 -1.2054727274809207  4.8740931166142563  7.8591193484922108
  1.6075052966354850  5.5704141948994526  7.8591687135558166
  4.4232040535151498  6.2656128872572729  7.8587807553999207
 -0.4019242656636173  7.6583220908782481  7.8590825188619267
  2.4120383436496011  8.3540525555722915  7.8587895664942291
  8.8445039162870867  0.4647968941776787 10.2755520864748000
  1.2063226009228931  1.1593650275684138 10.2755837754173047
  6.8329809483950861  2.5537984134984182 10.2740842034512951
 -0.8020720513989207  3.2481349076053885 10.2750322900062816
  2.0116191117973359  3.9466580717831454 10.2741042582928745
  0.0000248879312608  6.0342429676442970 10.2740922232280116
  2.8139995857314988  6.7326567697732100 10.2750272999893362
  0.8021774807534926  8.8200899111924222 10.2740493675852811
 -3.6188345293885122  8.5863811881476000 12.6917955534697704
 -0.4006763176303467  1.6241122117887199 12.6918090122397853
  2.4128925697573109  2.3195217483836097 12.6906455539266236
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  8.0402852802117337  3.7149694803866269 12.6901777835426568
  0.4027327597189356  4.4101647890427484 12.6904161343126347
  3.2142750878443667  5.1055579469870169 12.6902132084695189
 -1.6077677589304107  6.4974974552552647 12.6903966286473029
  1.2051982775833403  7.1949139773281612 12.6904219638344316
  4.0197617263688743  7.8922620508161572 12.6917823326009120
  7.2365291587633882  0.9296977153726051 12.6907325797777286
  5.6277923887529209  1.3932491412625354  7.8571225132595108
  6.4311102287952311  4.1771590027975964  7.8571674741332638
 -3.2148414737077249  6.9631804427554327  7.8587078568890183
 -2.0116813315394735  8.1219295943505312 10.2749759042997422
  4.0210524924150999  1.8568440441747116 10.2740789790561742
  4.8234102686626601  4.6405655624466551 10.2740810593326000
 -2.8136990261133432  5.3358516291346945 10.2741178146610803
  5.6267576264006030  7.4270248849843430 10.2755416321589372
  4.4230188736205900  0.2307521563163879 12.6901477739640463
  5.2259029450914527  3.0170448910076515 12.6906470746538069
  6.0280192813622273  5.8020892232561501 12.6906654145006303

Interface: O-a-SiO2(0001)/fcc(111)_sqrt13/Ag E_tot= -956.9233853 eV
 D3-zero damping= -23.4713226 eV, D3-BJ damping= -30.1391654 eV
Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O
Si  O  H Ag
 1.0000000000000000
    10.3858879861668498    0.0000000000000000    0.0000000000000000
    -5.1929439930834222    8.9944428368800970    0.0000000000000000
     0.0000000000000023    0.0000000000000039   37.1264016893996427
   2   5   3   6   3   7   2   2   5   3   6   3   7   2   2   5   3   6
3   7   2   2   5   3   6   3   7   2  39
Selective dynamics
Cartesian
  2.6778476832652180  0.1920890247303581  9.0169746245084816   F   F   F
 -1.3038961182772821  2.4807408929664447 10.8612336967246357   F   F   F
  2.4021363422036819  2.7413478597727914 11.6081185941916658   F   F   F
  3.6446545416015215  1.4769460860063122  9.5654178022134708   F   F   F
 -0.6561402831850477  3.9343139658965764 10.2987723773365900   F   F   F
  1.1555107375691265  3.5928563113098142  8.2518078419286880   F   F   F
 -0.2040663487150783  1.7972298652252008 11.9218080039603862   F   F   F
  2.7280965345798727 -0.0469069246184223 14.5050718430130097   F   F   F
  1.2778480028925316  2.1037212866817088 12.6701466762358947   F   F   F
 -1.2276107376852745  2.2855614160480786 16.2979587912671420   T   T   T
  2.6642127034952003  2.3582366081009840 17.1219952470057670   T   T   T
  3.7210411146187234  1.0724707616930507 15.1235075836287454   T   T   T
  1.8170158028103900  0.6288445269474858 13.2917821082657603   F   F   F
 -0.8502442929501448  3.7013351987940402 15.5695099331842979   T   T   T
  1.1063265906219368  3.2173921336172655 13.8903255655927040   F   F   F
  0.0280834737977514  1.7732345312725877 17.2041692848496233   T   T   T
  0.1351047045241522  4.3956904787956734 19.7472340159223876   T   T   T
  1.3675857372819986  2.1417475522194347 18.0641271497525970   T   T   T
  4.0860242344834408  2.2202926406786836 21.6573416765589180   T   T   T
  3.7622448356790557  0.9636498579510986 20.6729408627954285   T   T   T
  1.6347782683183523  0.9069112520277269 19.1043757897849034   T   T   T
 -0.7492818725397692  3.2353569136461098 20.4688366069324452   T   T   T
  1.1555522637219748  3.5992008523947536 18.7661657038095520   T   T   T
  0.1647481895550036  1.6003221913373005 22.4811589523233231   T   T   T
  2.8909127777899926  2.3375662182526624 22.7804024348028840   T   T   T
  1.4413596142545126  0.7118598035102008  8.0000000000000000   F   F   F
  1.2311570823942311  1.7287453318958153  8.0158744918591083   F   F   F
  2.0651055659662774  4.0168412792289496  8.0308754104330902   F   F   F
  0.0813756867235068  4.6893104431704069  9.0169746245084816   F   F   F
 -3.9003681148189928  6.9779623114064933 10.8612336967246357   F   F   F
 -0.1943356543380296  7.2385692782128412 11.6081185941916658   F   F   F
  1.0481825450598103  5.9741675044463607  9.5654178022134708   F   F   F
```

-3.2526122797267587	8.4315353843366250	10.2987723773365900	F	F	F
-1.4409612589725846	8.0900777297498632	8.2518078419286880	F	F	F
-2.8005383452567898	6.2944512836652491	11.9218080039603862	F	F	F
0.1316245380381616	4.4503144938216259	14.5050718430130097	F	F	F
-1.3186239936491795	6.6009427051217573	12.6701466762358947	F	F	F
-3.9179008248462202	6.8149284186301831	16.2929567061718146	T	T	T
-0.1642044645462331	7.0627094653680347	17.0055418317795066	T	T	T
1.0651034161178079	5.5905831593064548	15.1867280809115908	T	T	T
-0.7794561937313210	5.1260659453875350	13.2917821082657603	F	F	F
-3.4567106731302375	8.2209072158186025	15.5836796012810570	T	T	T
-1.4901454059197743	7.7146135520573145	13.8903255655927040	F	F	F
-2.7278800874226437	6.2952570572110007	17.2800502338458948	T	T	T
-2.4904454784385015	8.9696679236980987	19.9364931744022265	T	T	T
-1.3453018542306765	6.6818332452648326	18.0582166960965438	T	T	T
1.1189580042823688	6.6758262487005684	21.6458906394421220	T	T	T
1.0325072176552517	5.2682929702083170	20.7942948201469733	T	T	T
-0.8761388173476675	5.3991110229969443	18.9494001220690151	T	T	T
-3.2682441404796094	8.0250051403879343	21.0084974091172967	T	T	T
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Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Ag E_tot= -880.85276547 eV
 D3-zero damping= -8.1546242 eV, D3-BJ damping= -11.6576986 eV
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Selective dynamics
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3.6299728649508691	7.9872280672640175	19.0095469816106757	T	T	T
2.6566586064912716	6.2730725238728233	22.4962596564354165	T	T	T
5.3026083744357653	7.2021139243442152	22.7315416958359684	T	T	T
4.3656935454879688	6.9001048228795048	22.6401008450381056	T	T	T
2.6901088002074305	5.3382370017302305	22.7825131846704849	T	T	T
4.0378316107962267	5.2090812219502496	8.0000000000000000	F	F	F
3.8276290789359448	6.2259667503358642	8.0158744918591047	F	F	F
4.6615775625079916	8.5140626976689973	8.0308754104330866	F	F	F

```
Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Ag E_tot= -109.60448298 eV
 D3-zero damping= -12.4169229 eV, D3-BJ damping= -15.7714089 eV
Ag
 1.0000000000000000
    10.3858879861668498    0.0000000000000000    0.0000000000000000
    -5.1929439930834222    8.9944428368800970    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000323980098436  0.0000161467290190  7.8875646103515074
  2.7954954851858491  0.6924502935560881  7.8886013067205907
  8.3884076626024644  2.0747301297338936  7.8885769843793812
  0.7982261246468355  2.7671885389912565  7.8885278624426798
  3.5955832210211884  3.4591520783860181  7.8868784695095666
 -1.1979382834132410  4.8431652720040486  7.8883943167739652
  1.5976283143044490  5.5354403544628665  7.8884392556723766
  4.3949946206649910  6.2272434664654215  7.8886074369616095
 -0.3996679505562832  7.6102898181512826  7.8884756891324184
  2.3975343621723506  8.3022201236126385  7.8885328048476220
  8.7879530794437937  0.4611170599018328 10.2757286857974268
  1.1984990810770146  1.1533803914758975 10.2758796148622960
  6.7910345903884970  2.5371863201873297 10.2740530206427021
 -0.7985438201991050  3.2286294989510007 10.2750428378317906
  1.9983064156203536  3.9222691858811198 10.2741315478896063
  0.0000355203946032  5.9962885281451301 10.2739976319286210
  2.7963532453181434  6.6886192538372979 10.2750326375465484
  0.7970520609008078  8.7638399534066274 10.2740748339834713
 -3.5953713681917954  8.5328266405236270 12.6619918293677944
 -0.3988468181636216  1.6142929138343054 12.6620297287616328
  2.3978114057799544  2.3059039230144740 12.6610992827343871
  7.9891546006726664  3.6911646274855783 12.6605041226791037
  0.4007187800970778  4.3818255575604033 12.6610270019424149
  3.1948066202481309  5.0731230071890643 12.6605212625088708
 -1.5984196482039481  6.4564853729678742 12.6610335620727952
  1.1979078015087026  7.1504629973387601 12.6610222602256286
  3.9945337900377815  7.8418013397661541 12.6619124713693978
  7.1900598598672012  0.9235821430006279 12.6611798839436176
  5.5924133135037390  1.3843044901982020  7.8868945316795731
  6.3908450560240286  4.1509839940171185  7.8869312230171760
 -3.1955782392037957  6.9196245227568465  7.8884071145575199
 -1.9975067988823123  8.0717883366692948 10.2749943396593899
  3.9947433101423329  1.8445795414764581 10.2740320327309522
  4.7931140788152904  4.6125961219519844 10.2740618468379967
 -2.7952520502311660  5.3026229320910412 10.2741223432374369
  5.5924221223937751  7.3799155629421564 10.2757637578500240
  4.3951690162679364  0.2300774298767013 12.6604592919816632
  5.1930109845758716  2.9980958043038552 12.6614176409864143
  5.9910317637272481  5.7648610201565775 12.6611915316042296

Interface: O-a-SiO2(0001)/fcc(111)_sqrt13/Cu E_tot= -983.2756052 eV
 D3-zero damping= -25.6458855 eV, D3-BJ damping= -33.5646022 eV
Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O
Si  O  H Cu
 1.0000000000000000
     9.0995808326891421    0.0000000000000000    0.0000000000000000
    -4.5497904163445693    7.8804681648987538    0.0000000000000000
     0.0000000000000023    0.0000000000000039   36.9506544979083813
   2   5   3   6   3   7   2   2   5   3   6   3   7   2   2   5   3   6
3   7   2   2   5   3   6   3   7   2  39
Selective dynamics
Cartesian
  2.3461923991435722  0.1682985229509905  9.0169746245084816   F   F   F
```

-1.1424067100951616	2.1734975681012472	10.8612336967246357	F	F	F
2.1046283039193439	2.4018279875294963	11.6081185941916658	F	F	F
3.1932588385994021	1.2940241906169909	9.5654178022134708	F	F	F
-0.5748763661208594	3.4470435269027706	10.2987723773365900	F	F	F
1.0123990720442182	3.1478758935727056	8.2518078419286880	F	F	F
-0.1787924381466321	1.5746403634741648	11.9218080039603862	F	F	F
2.3902178580062605	-0.0410974345907345	14.5050718430130097	F	F	F
1.1195846912366436	1.8431723818999302	12.6701466762358947	F	F	F
-1.3021341224915708	2.1117344734865044	16.4978267109460361	T	T	T
1.8226936010777628	2.3789027180020681	17.0973250701441444	T	T	T
3.3504695579786681	1.0512975483304856	15.2290761200671980	T	T	T
1.5919757842534736	0.5509612285222355	13.2917821082657603	F	F	F
-0.7901673799859872	3.4737544606736832	15.7834840975406365	T	T	T
0.9693064523829126	2.8189134938970022	13.8903255655927040	F	F	F
-0.4445421253158600	1.4899712380840711	17.7360257930875989	T	T	T
-0.1410046715732057	4.0566193781323250	20.0742881498068613	T	T	T
0.9925864632393407	1.8471358045166284	18.3934606098360121	T	T	T
3.2693261150331656	1.5911316986513588	22.1778029650892705	T	T	T
3.6855047346151872	0.6000963687067888	20.9690530746465420	T	T	T
1.6134594141450225	0.5492748896396010	19.1072052699164097	T	T	T
-1.2688829523718401	3.5159556733770572	21.1175740157843954	T	T	T
0.9157114350533222	2.9269590533917111	19.5997498610325707	T	T	T
0.3101240554954504	2.8184035181522775	23.1069950049781987	T	T	T
2.1332463412974834	0.9539578740700058	23.1567706755434024	T	T	T
1.2628451545358188	0.6236949437747595	8.0000000000000000	F	F	F
1.0786765083453167	1.5146377380222280	8.0158744918591083	F	F	F
1.8093392736928473	3.5193497138723218	8.0308754104330902	F	F	F
0.0712971909712871	4.1085326054003675	9.0169746245084816	F	F	F
-3.4173019182674467	6.1137316505506245	10.8612336967246357	F	F	F
-0.1702669042529412	6.3420620699788737	11.6081185941916658	F	F	F
0.9183636304271171	5.2342582730663683	9.5654178022134708	F	F	F
-2.8497715742931446	7.3872776093521466	10.2987723773365900	F	F	F
-1.2624961361280667	7.0881099760220829	8.2518078419286880	F	F	F
-2.4536876463189174	5.5148744459235415	11.9218080039603862	F	F	F
0.1153226498339757	3.8991366478586422	14.5050718430130097	F	F	F
-1.1553105169356412	5.7834064643493068	12.6701466762358947	F	F	F
-3.7406329307643400	6.0897469194877161	16.3476254985923717	T	T	T
-0.7519692097499112	6.1165962187459932	16.5572452556773797	T	T	T
1.1642411298032218	4.9950981301101924	15.1266161153985834	T	T	T
-0.6829194239188113	4.4911953109716123	13.2917821082657603	F	F	F
-3.2241429874287570	7.4824160319302822	15.7065702113487813	T	T	T
-1.3055887557893722	6.7591475763463800	13.8903255655927040	F	F	F
-2.9869585582944449	5.6710568514728568	17.7323534634437934	T	T	T
-1.8942309808804056	7.6377620378635527	20.0489843800920795	T	T	T
-1.3928197547003489	5.7341220052583717	17.9963094018997189	T	T	T
1.1321182086580703	6.0486855055893249	22.1800956264361631	T	T	T
0.6771209878761846	5.2148024947816243	20.8555877126509550	T	T	T
-0.9288881694918746	4.3546234321572364	18.6825785188485867	T	T	T
-2.6859666869162817	6.6318428052502432	21.0068815872860313	T	T	T
-0.9150121707806647	6.8582622488352962	19.0454421172799577	T	T	T
-2.7530628630588674	4.9699745242477844	23.0300124094954768	T	T	T
-0.1004573045710156	6.6221551136088772	23.1130578525540216	T	T	T
-1.0120500536364661	4.5639290262241365	8.0000000000000000	F	F	F
-1.1962186998269682	5.4548718204716051	8.0158744918591083	F	F	F
-0.4655559344794373	7.4595837963216987	8.0308754104330902	F	F	F
6.8959828154881437	0.1682985229509905	9.0169746245084816	F	F	F
3.4073837062494094	2.1734975681012472	10.8612336967246357	F	F	F
6.6544187202639158	2.4018279875294963	11.6081185941916658	F	F	F
7.7430492549439727	1.2940241906169909	9.5654178022134708	F	F	F
3.9749140502237119	3.4470435269027706	10.2987723773365900	F	F	F
5.5621894883887899	3.1478758935727056	8.2518078419286880	F	F	F
4.3709979781979396	1.5746403634741648	11.9218080039603862	F	F	F
6.9400082743508325	-0.0410974345907345	14.5050718430130097	F	F	F

5.6693751075812147	1.8431723818999302	12.6701466762358947	F	F	F
3.2900458305837952	2.0836827586856761	16.4810789521259409	T	T	T
6.3828485457277164	2.4937655972672985	17.2044248971083000	T	T	T
7.8497482074841649	1.0853025999532968	15.2372450758581106	T	T	T
6.1417662005980445	0.5509612285222355	13.2917821082657603	F	F	F
3.7748962420377361	3.4659709457668253	15.7930645861159888	T	T	T
5.5190968687274840	2.8189134938970022	13.8903255655927040	F	F	F
4.1376594647758722	1.5456167737603852	17.7710264052250118	T	T	T
3.9699503877277982	3.8571454947517148	20.3078607580862212	T	T	T
5.5261030326150058	1.9858916577978252	18.5035803848112472	T	T	T
8.2080980041766498	2.2864678638771858	22.1202276774509627	T	T	T
8.3865325426696433	1.0399428856152406	21.0666768080023736	T	T	T
6.2446625743084629	0.7902351837322823	19.2985025674049346	T	T	T
3.0436714951789843	2.9852262099742557	21.3540139412708250	T	T	T
5.2542129086942309	3.0641710251751606	19.7002601730284042	T	T	T
4.4780358835655019	1.7859379810159577	23.3045166262149870	T	T	T
7.0225653805113666	2.0067862952995101	23.2231134569873880	T	T	T
5.8126355708803903	0.6236949437747595	8.0000000000000000	F	F	F
5.6284669246898877	1.5146377380222280	8.0158744918591083	F	F	F
6.3591296900374195	3.5193497138723218	8.0308754104330902	F	F	F
4.6210876073158582	4.1085326054003675	9.0169746245084816	F	F	F
1.1324884980771248	6.1137316505506245	10.8612336967246357	F	F	F
4.3795235120916294	6.3420620699788737	11.6081185941916658	F	F	F
5.4681540467716889	5.2342582730663683	9.5654178022134708	F	F	F
1.7000188420514268	7.3872776093521466	10.2987723773365900	F	F	F
3.2872942802165048	7.0881099760220829	8.2518078419286880	F	F	F
2.0961027700256545	5.5148744459235415	11.9218080039603862	F	F	F
4.6651130661785469	3.8991366478586422	14.5050718430130097	F	F	F
3.3944798994089300	5.7834064643493068	12.6701466762358947	F	F	F
0.8460548946666643	6.0861384310611042	16.2838596959730779	T	T	T
3.8142356985536061	6.1507397265613450	16.8459885603161652	T	T	T
5.6328475767836128	5.0469397604669526	15.1332884650024830	T	T	T
3.8668709924257594	4.4911953109716123	13.2917821082657603	F	F	F
1.3314252493606615	7.4909761093755272	15.6834150989212926	T	T	T
3.2442016605551984	6.7591475763463800	13.8903255655927040	F	F	F
1.4857837004739274	5.8223195713579452	17.7567266001607607	T	T	T
2.7192493616536733	7.9694244629605411	20.3377643666334755	T	T	T
3.0356720138153777	5.8219388032781838	18.2486221234183077	T	T	T
5.4224364511340468	5.9968854128651623	22.0989019873412680	T	T	T
4.4017159681650089	5.0821161525893599	21.2427767358054709	T	T	T
3.2262113939326489	4.3697948927173131	18.9518916753101472	T	T	T
1.9163202126828527	7.3293332618781069	21.5821299577460373	T	T	T
3.4696329599348275	6.8960986791137380	19.3814820665236880	T	T	T
2.1221788141220386	5.1960682388957311	23.2033304722894727	T	T	T
4.6012103301219316	7.0357402248988006	23.0159006653836613	T	T	T
3.5377403627081052	4.5639290262241365	8.0000000000000000	F	F	F
3.3535717165176036	5.4548718204716051	8.0158744918591083	F	F	F
4.0842344818651339	7.4595837963216987	8.0308754104330902	F	F	F
-0.0816942476266760	-0.9190523982468397	24.8643944013787213	T	T	T
2.3744338940556182	-0.3180954102465275	24.7118271073336118	T	T	T
7.2701140452727904	0.8361314917163378	24.7418948996734258	T	T	T
0.6888527843577733	1.4779144342691524	24.6048359220053641	T	T	T
3.1902504154824625	2.1653825137857168	24.8416478862301524	T	T	T
-1.1574618382347310	3.2887331327259699	24.7312734726379624	T	T	T
1.3361403593731052	3.9133672072109484	24.5639498241414671	T	T	T
3.7746445720746364	4.5552316727493141	24.7659585864636078	T	T	T
-0.4917473056197299	5.7108376519716186	24.7726606343833673	T	T	T
2.0511843563161571	6.3425723801435474	24.8339283261655517	T	T	T
7.6090595104018979	-0.5019378290293579	26.8379019926107354	T	T	T
0.9956871425820927	0.1089198942171175	26.8069500842790802	T	T	T
5.8526276455908768	1.3107286000790281	26.7147271283661247	T	T	T
-0.7494139279898479	1.8814851723243604	26.7516842581865752	T	T	T
1.6849390889232438	2.5272781950339529	26.7319609308217778	T	T	T

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 -0.0814262044653288  4.3209728908473135 26.7491175524303095   T   T   T
  2.3634621410947041  4.9105938084350305 26.8126427864909544   T   T   T
  0.6202869089737625  6.7835801136489682 26.7888177443933913   T   T   T
 -3.2191891817783236  6.5692938364717159 28.9501729279029796   T   T   T
 -0.4145914306788749  0.4965980848007250 28.9013554987104655   T   T   T
  2.0339913085748260  1.1135348685731055 28.8779679474015119   T   T   T
  6.9385510442456573  2.2936230784960521 28.8563515510730006   T   T   T
  0.2803957454854087  2.9189600415208821 28.8389710158741792   T   T   T
  2.7246963324737816  3.5246763707133963 28.9024283295635840   T   T   T
 -1.4657043273604629  4.7341402773954968 28.9239528761643712   T   T   T
  0.9648877592574475  5.3455060860877675 28.8472645070992648   T   T   T
  3.4151032313445882  5.9519319790231862 28.9273018981387651   T   T   T
  6.2182738471265324 -0.1041347309776700 28.9034423229798065   T   T   T
  4.8635212909460419  0.2119540049748380 24.5837561980717361   T   T   T
  5.4468024641158364  3.3668372026492164 23.3736148269193933   T   T   T
 -2.8836714422258414  5.1434186006846003 24.9457713285581448   T   T   T
 -1.8175932750658630  6.1723386651554017 26.8625277097997532   T   T   T
  3.4484330706465625  0.6929035621909589 26.7897667740649865   T   T   T
  4.1597935612823154  3.1462140422437965 26.8202672078554372   T   T   T
 -2.5068182165329644  3.6972526675244461 26.8393392042105567   T   T   T
  4.8155781978803560  5.5543397671700685 26.9008480047085428   T   T   T
  3.7816625102607997 -0.7032956850460935 28.9114298719551464   T   T   T
  4.4859191780890733  1.7107645271777547 28.8704424934427628   T   T   T
  5.1882148380593724  4.1287066494657108 28.9351324737252789   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Cu E_tot= -868.27988442 eV
 D3-zero damping= -10.7239259 eV, D3-BJ damping= -15.3552704 eV
Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H
O  H Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     9.0995808326891421    0.0000000000000000    0.0000000000000000
    -4.5497904163445693    7.8804681648987538    0.0000000000000000
     0.0000000000000019    0.0000000000000033   31.1539601278806977
   2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.3461923991435722  0.1682985229509905  9.0169746245084816   F   F   F
 -1.1424067100951616  2.1734975681012472 10.8612336967246357   F   F   F
  2.1046283039193439  2.4018279875294963 11.6081185941916623   F   F   F
  3.1932588385994021  1.2940241906169909  9.5654178022134708   F   F   F
 -0.5748763661208594  3.4470435269027706 10.2987723773365900   F   F   F
  1.0123990720442182  3.1478758935727056  8.2518078419286844   F   F   F
 -0.1787924381466321  1.5746403634741648 11.9218080039603862   F   F   F
  2.3902178580062605 -0.0410974345907345 14.5050718430130097   F   F   F
  1.1195846912366436  1.8431723818999302 12.6701466762358947   F   F   F
 -1.3574851454633741  2.1201483287480309 16.3995139080737147   T   T   T
  1.6692456494545516  2.2799275151875595 16.9257187474738906   T   T   T
  3.3765411827949308  1.0662987410989238 15.1800581916088433   T   T   T
  1.5919757842534736  0.5509612285222355 13.2917821082657603   F   F   F
 -0.8715332043799769  3.5133486542424546 15.7420757339254376   T   T   T
  0.9693064523829126  2.8189134938970022 13.8903255655927005   F   F   F
 -0.6092486195273922  1.6992383005409211 17.7766126204398134   T   T   T
 -0.2365035403694356  3.6243306016191692 20.2194256772317047   T   T   T
  0.9094770877419294  1.8997261684891498 18.3127847362923681   T   T   T
  3.0823089557253884  1.7151443913723978 22.1443099661891800   T   T   T
  2.3105735210691978  0.3558433007211005 21.6804395270407255   T   T   T
  1.2659514097469440  0.5460755462188590 19.1022518827743220   T   T   T
 -1.1035180400111793  2.3358530884372519 20.6856988105583390   T   T   T
  1.0711599801878087  3.0878437640688978 19.4197972416491318   T   T   T
 -0.1612222533303482  1.3480127847321357 23.0593464483075579   T   T   T
  2.1071225994772629  2.6604783132863319 23.0531303863761714   T   T   T
  1.1837361498025742  2.2671760806600760 23.1505203696345170   T   T   T
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-0.0403315077206389	0.3520784779372446	23.1539601278806941	T	T	T
1.2628451545358188	0.6236949437747595	8.0000000000000000	F	F	F
1.0786765083453167	1.5146377380222280	8.0158744918591047	F	F	F
1.8093392736928473	3.5193497138723218	8.0308754104330866	F	F	F
0.0712971909712876	4.1085326054003675	9.0169746245084816	F	F	F
-3.4173019182674462	6.1137316505506245	10.8612336967246357	F	F	F
-0.1702669042529408	6.3420620699788728	11.6081185941916623	F	F	F
0.9183636304271174	5.2342582730663683	9.5654178022134708	F	F	F
-2.8497715742931442	7.3872776093521475	10.2987723773365900	F	F	F
-1.2624961361280664	7.0881099760220820	8.2518078419286844	F	F	F
-2.4536876463189166	5.5148744459235415	11.9218080039603862	F	F	F
0.1153226498339759	3.8991366478586422	14.5050718430130097	F	F	F
-1.1553105169356410	5.7834064643493068	12.6701466762358947	F	F	F
-3.6323803536356589	6.0603824111974074	16.3995139080737147	T	T	T
-0.6056495587177331	6.2201615976369364	16.9257187474738906	T	T	T
1.1016459746226461	5.0065328235483006	15.1800581916088433	T	T	T
-0.6829194239188110	4.4911953109716123	13.2917821082657603	F	F	F
-3.1464284125522615	7.4535827366918319	15.7420757339254376	T	T	T
-1.3055887557893722	6.7591475763463791	13.8903255655927005	F	F	F
-2.8841438276996767	5.6394723829902977	17.7766126204398134	T	T	T
-2.5113987485417204	7.5645646840685465	20.2194256772317047	T	T	T
-1.3654181204303553	5.8399602509385264	18.3127847362923681	T	T	T
0.8074137475531038	5.6553784738217745	22.1443099661891800	T	T	T
0.0356783128969131	4.2960773831704770	21.6804395270407255	T	T	T
-1.0089437984253407	4.4863096286682360	19.1022518827743220	T	T	T
-3.3784132481834641	6.2760871708866288	20.6856988105583390	T	T	T
-1.2037352279844760	7.0280778465182747	19.4197972416491318	T	T	T
-2.4361174615026329	5.2882468671815124	23.0593464483075579	T	T	T
-0.1677726086950218	6.6007123957357088	23.0531303863761714	T	T	T
-1.0911590583697104	6.2074101631094525	23.1505203696345170	T	T	T
-2.3152267158929236	4.2923125603866215	23.1539601278806941	T	T	T
-1.0120500536364658	4.5639290262241365	8.0000000000000000	F	F	F
-1.1962186998269679	5.4548718204716051	8.0158744918591047	F	F	F
-0.4655559344794373	7.4595837963216987	8.0308754104330866	F	F	F
6.8959828154881428	0.1682985229509905	9.0169746245084816	F	F	F
3.4073837062494094	2.1734975681012472	10.8612336967246357	F	F	F
6.6544187202639149	2.4018279875294963	11.6081185941916623	F	F	F
7.7430492549439727	1.2940241906169909	9.5654178022134708	F	F	F
3.9749140502237115	3.4470435269027706	10.2987723773365900	F	F	F
5.5621894883887890	3.1478758935727056	8.2518078419286844	F	F	F
4.3709979781979387	1.5746403634741648	11.9218080039603862	F	F	F
6.9400082743508316	-0.0410974345907345	14.5050718430130097	F	F	F
5.6693751075812147	1.8431723818999302	12.6701466762358947	F	F	F
3.1923052708811968	2.1201483287480309	16.3995139080737147	T	T	T
6.2190360657991226	2.2799275151875595	16.9257187474738906	T	T	T
7.9263315991395018	1.0662987410989238	15.1800581916088433	T	T	T
6.1417662005980445	0.5509612285222355	13.2917821082657603	F	F	F
3.6782572119645942	3.5133486542424546	15.7420757339254376	T	T	T
5.5190968687274840	2.8189134938970022	13.8903255655927005	F	F	F
3.9405417968171790	1.6992383005409211	17.7766126204398134	T	T	T
4.3132868759751357	3.6243306016191692	20.2194256772317047	T	T	T
5.4592675040865002	1.8997261684891498	18.3127847362923681	T	T	T
7.6320993720699590	1.7151443913723978	22.1443099661891800	T	T	T
6.8603639374137693	0.3558433007211005	21.6804395270407255	T	T	T
5.8157418260915152	0.5460755462188590	19.1022518827743220	T	T	T
3.4462723763333916	2.3358530884372519	20.6856988105583390	T	T	T
5.6209503965323799	3.0878437640688978	19.4197972416491318	T	T	T
4.3885681630142228	1.3480127847321357	23.0593464483075579	T	T	T
6.6569130158218339	2.6604783132863319	23.0531303863761714	T	T	T
5.7335265661471455	2.2671760806600760	23.1505203696345170	T	T	T
4.5094589086239321	0.3520784779372446	23.1539601278806941	T	T	T
5.8126355708803903	0.6236949437747595	8.0000000000000000	F	F	F
5.6284669246898877	1.5146377380222280	8.0158744918591047	F	F	F

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  6.3591296900374186  3.5193497138723218  8.0308754104330866   F   F   F
  4.6210876073158591  4.1085326054003675  9.0169746245084816   F   F   F
  1.1324884980771248  6.1137316505506245 10.8612336967246357   F   F   F
  4.3795235120916303  6.3420620699788728 11.6081185941916623   F   F   F
  5.4681540467716889  5.2342582730663683  9.5654178022134708   F   F   F
  1.7000188420514271  7.3872776093521475 10.2987723773365900   F   F   F
  3.2872942802165044  7.0881099760220820  8.2518078419286844   F   F   F
  2.0961027700256545  5.5148744459235415 11.9218080039603862   F   F   F
  4.6651130661785469  3.8991366478586422 14.5050718430130097   F   F   F
  3.3944798994089300  5.7834064643493068 12.6701466762358947   F   F   F
  0.9174100627089123  6.0603824111974074 16.3995139080737147   T   T   T
  3.9441408576268380  6.2201615976369364 16.9257187474738906   T   T   T
  5.6514363909672172  5.0065328235483006 15.1800581916088433   T   T   T
  3.8668709924257598  4.4911953109716123 13.2917821082657603   F   F   F
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  3.1843722959142156  5.8399602509385264 18.3127847362923681   T   T   T
  5.3572041638976753  5.6553784738217745 22.1443099661891800   T   T   T
  4.5854687292414837  4.2960773831704770 21.6804395270407255   T   T   T
  3.5408466179192306  4.4863096286682360 19.1022518827743220   T   T   T
  1.1713771681611072  6.2760871708866288 20.6856988105583390   T   T   T
  3.3460551883600953  7.0280778465182747 19.4197972416491318   T   T   T
  2.1136729548419382  5.2882468671815124 23.0593464483075579   T   T   T
  4.3820178076495493  6.6007123957357088 23.0531303863761714   T   T   T
  3.4586313579748609  6.2074101631094525 23.1505203696345170   T   T   T
  2.2345637004516474  4.2923125603866215 23.1539601278806941   T   T   T
  3.5377403627081052  4.5639290262241365  8.0000000000000000   F   F   F
  3.3535717165176031  5.4548718204716051  8.0158744918591047   F   F   F
  4.0842344818651339  7.4595837963216987  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Cu E_tot= -145.76161747 eV
 D3-zero damping= -12.2185282 eV, D3-BJ damping= -15.3357517 eV
Cu
 1.0000000000000000
     9.0995808326891421    0.0000000000000000    0.0000000000000000
    -4.5497904163445693    7.8804681648987538    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000156215270264  0.0000282465690322  8.2053024337537526
  2.4493240706182196  0.6056713199316976  8.2049046118465334
  7.3504695036120387  1.8183429543580807  8.2049933642149657
  0.7001176040599204  2.4240493096732174  8.2051052892559611
  3.1508404953214137  3.0314994079203665  8.2036611019753991
 -1.0496386470811279  4.2444281805489981  8.2046426589648629
  1.3988827833441528  4.8491833642054560  8.2046681032109472
  3.8496996851589094  5.4565288388740374  8.2049314165021237
 -0.3491423866165154  6.6673563048046738  8.2046006326582948
  2.1004768915564145  7.2748222582234732  8.2050969138215066
  7.7009135487087503  0.4044359517752665 10.2756754694018593
  1.0497834034087608  1.0090824456405003 10.2756305778561945
  5.9493007475137833  2.2217907314696403 10.2740807374903138
 -0.7007555001912739  2.8298286092537550 10.2747283017980156
  1.7493419904761172  3.4354393403185894 10.2741831117347040
  0.0000745324189116  5.2536481338065766 10.2745747907942526
  2.4495681900757722  5.8586418827739868 10.2747293445966044
  0.6999421766492492  7.6776996896355323 10.2741461193528991
 -3.1503495148943697  7.4758697322515362 12.3458230632283925
 -0.3492584398519966  1.4141718651800339 12.3458211603724894
  2.1003217488172385  2.0214904126046589 12.3440561674857889
  6.9992561514341682  3.2332380063278090 12.3440973530973377
```

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  0.3501032286302939  3.8394527113482706 12.3443851652124028
  2.7999835051290582  4.4447723105843124 12.3440853522806897
 -1.3996774631086242  5.6575529073886859 12.3443792304513806
  1.0497331664169220  6.2638591776251511 12.3443779330138952
  3.4997941572436737  6.8708696878299271 12.3458669849129823
  6.2988189753007440  0.8081029181289996 12.3440940907898504
  4.8988672293895306  1.2129691607406665  8.2036506132511615
  5.5997340275960559  3.6360150088398351  8.2036631599358039
 -2.8005537456569565  6.0621668365315262  8.2050985270287011
 -1.7486107045807255  7.0724555609210755 10.2747000758448088
  3.4993043150038989  1.6172953425276095 10.2740403824412869
  4.2008415060626012  4.0413386344639246 10.2740562360083398
 -2.4492085112619391  4.6476972863990733 10.2741697487456598
  4.8987098112604741  6.4668919095507995 10.2756516120398409
  3.8503997512442183  0.2023840648819068 12.3440702562890259
  4.5498220340550954  2.6268114973318477 12.3453269031943567
  5.2503638023903276  5.0507756607925991 12.3440679013400736

Interface: O-a-SiO2(0001)/fcc(111)_sqrt13/Pt E_tot= -1091.99640007 eV
 D3-zero damping= -30.867312 eV, D3-BJ damping= -35.8824608 eV
Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O
Si  O  H Pt
 1.0000000000000000
     9.9890116653035843    0.0000000000000000    0.0000000000000000
    -4.9945058326517895    8.6507378608520060    0.0000000000000000
     0.0000000000000023    0.0000000000000039   37.2220922030863903
   2   5   3   6   3   7   2   2   5   3   6   3   7   2   2   5   3   6
3   7   2   2   5   3   6   3   7   2  39
Selective dynamics
Cartesian
  2.5755189909298060  0.1847487197400928  9.0169746245084816   F   F   F
 -1.2540702877947054  2.3859442496821237 10.8612336967246357   F   F   F
  2.3103434175182311  2.6365926328492870 11.6081185941916658   F   F   F
  3.5053812231125305  1.4205074907212190  9.5654178022134708   F   F   F
 -0.6310671703315774  3.7839718811383261 10.2987723773365900   F   F   F
  1.1113551631150940  3.4555623605063581  8.2518078419286880   F   F   F
 -0.1962683538014117  1.7285522540660792 11.9218080039603862   F   F   F
  2.6238476810349494 -0.0451144685770741 14.5050718430130097   F   F   F
  1.2290175500043494  2.0233317075246826 12.6701466762358947   F   F   F
 -1.3086721237468082  2.2442548030757798 16.3275765013001433   T   T   T
  2.2506147514556041  2.4423123812069747 16.9755201259271473   T   T   T
  3.6054887067165962  1.0659282355136601 15.1694100716467197   T   T   T
  1.7475821108882081  0.6048144678343575 13.2917821082657603   F   F   F
 -0.8478046053422110  3.6353962178117349 15.6287629294464701   T   T   T
  1.0640504917901330  3.0944458092909142 13.8903255655927040   F   F   F
 -0.2549726971343172  1.7635725132819264 17.4745568472507742   T   T   T
  0.0226451757403924  4.1790101097851018 19.8197659276122558   T   T   T
  1.2167235557266038  1.9837782197529024 18.1359798268181933   T   T   T
  4.1864387853993783  1.9061791883964083 21.7672117063216106   T   T   T
  3.7052739768891043  0.9861995804120479 20.5236457740249918   T   T   T
  1.6907824633536457  0.5905105734923092 18.8301832174640680   T   T   T
 -1.1319414469290088  3.3056423391275453 20.5543783767685220   T   T   T
  1.1638532218977591  3.1681961287285643 19.2540567037515657   T   T   T
  0.4294312916677772  2.1237149020342034 22.4274336955229572   T   T   T
  2.9670713343693524  1.8544347634622034 22.8993924913861449   T   T   T
  1.3862808861276410  0.6846574785704490  7.9999999999999991   F   F   F
  1.1841108313739839  1.6626847227359456  8.0158744918591083   F   F   F
  1.9861916107699016  3.8633455752010031  8.0308754104330902   F   F   F
  0.0782660746039111  4.5101176501660962  9.0169746245084816   F   F   F
 -3.7513232041205997  6.7113131801081272 10.8612336967246357   F   F   F
 -0.1869094988076638  6.9619615632752909 11.6081185941916658   F   F   F
  1.0081283067866353  5.7458764211472220  9.5654178022134708   F   F   F
 -3.1283200866574723  8.1093408115643282 10.2987723773365900   F   F   F
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-1.3858977532108010	7.7809312909323616	8.2518078419286880	F	F	F
-2.6935212701273068	6.0539211844920819	11.9218080039603862	F	F	F
0.1265947647090548	4.2802544618489291	14.5050718430130097	F	F	F
-1.2682353663215455	6.3487006379506861	12.6701466762358947	F	F	F
-3.8742492515507121	6.5740600100009923	16.3127332706020560	T	T	T
-0.3831307347601674	6.9521642811293214	16.9263219623981485	T	T	T
1.0437718806305931	5.4299411815734429	15.2080015066553642	T	T	T
-0.7496708054376867	4.9301833982603611	13.2917821082657603	F	F	F
-3.3818435430322795	7.9805558051627967	15.6383563829146333	T	T	T
-1.4332024245357617	7.4198147397169176	13.8903255655927040	F	F	F
-2.8206385632826527	6.0645113478176151	17.4378647522177950	T	T	T
-2.3698393195943042	8.5580245303551727	19.9804330363827383	T	T	T
-1.3580679384811754	6.3306105528103007	18.0744715405585623	T	T	T
0.8823789167659053	6.5493514838541342	21.7394036767474574	T	T	T
0.7103544113029726	5.1994498072083086	20.8655263370469122	T	T	T
-0.7057825827762635	4.9398457200847856	18.5882686665046997	T	T	T
-3.3278929786460267	8.0181377136581951	21.1825025478866635	T	T	T
-1.5080699782380345	7.3369930597123032	19.3398137537134645	T	T	T
-2.8925102853232487	5.7885470592874242	22.6909971772329655	T	T	T
-0.4762611669586189	7.0299474073088195	22.5016339277491788	T	T	T
-1.1109720301982537	5.0100264089964526	7.9999999999999991	F	F	F
-1.3131420849519109	5.9880536531619493	8.0158744918591083	F	F	F
-0.5110613055559931	8.1887145056270061	8.0308754104330902	F	F	F
7.5700248235815986	0.1847487197400928	9.0169746245084816	F	F	F
3.7404355448570872	2.3859442496821237	10.8612336967246357	F	F	F
7.3048492501700233	2.6365926328492870	11.6081185941916658	F	F	F
8.4998870557643222	1.4205074907212190	9.5654178022134708	F	F	F
4.3634386623202150	3.7839718811383261	10.2987723773365900	F	F	F
6.1058609957668866	3.4555623605063581	8.2518078419286880	F	F	F
4.7982374788503810	1.7285522540660792	11.9218080039603862	F	F	F
7.6183535136867420	-0.0451144685770741	14.5050718430130097	F	F	F
6.2235233826561407	2.0233317075246826	12.6701466762358947	F	F	F
3.7131614254748997	2.2173720627052256	16.3169567373035029	T	T	T
7.2360925253549153	2.5464246489738542	16.9947355826739539	T	T	T
8.5733343753446700	1.0716676420399092	15.1997402203407734	T	T	T
6.7420879435400005	0.6048144678343575	13.2917821082657603	F	F	F
4.1604286912935802	3.6345756237721170	15.6495601752498512	T	T	T
6.0585563244419252	3.0944458092909142	13.8903255655927040	F	F	F
4.7721714751382791	1.7475704410839059	17.4647043067787777	T	T	T
4.9234842494047699	4.3439260609125672	19.9775549624592230	T	T	T
6.1879990826423530	2.1545772200389295	18.1675208093175264	T	T	T
8.9255474507531147	2.2340815837349455	21.7724649267617991	T	T	T
8.4000764215069132	0.8111533653032617	21.1788594122114304	T	T	T
6.7709059271948773	0.9133344926692433	19.0203659035000676	T	T	T
4.3014309027470112	3.4426404262394406	21.1938507759201649	T	T	T
5.9781700784978167	3.4347960944238363	19.1455785210773506	T	T	T
5.5402264478607117	1.3569376707317453	22.4954174625028998	T	T	T
7.9362434252051770	2.8831844633543016	22.9496500326735458	T	T	T
6.3807867187794329	0.6846574785704490	7.9999999999999991	F	F	F
6.1786166640257756	1.6626847227359456	8.0158744918591083	F	F	F
6.9806974434216942	3.8633455752010031	8.0308754104330902	F	F	F
5.0727719072557038	4.5101176501660962	9.0169746245084816	F	F	F
1.2431826285311920	6.7113131801081272	10.8612336967246357	F	F	F
4.8075963338441285	6.9619615632752909	11.6081185941916658	F	F	F
6.0026341394384284	5.7458764211472220	9.5654178022134708	F	F	F
1.8661857459943201	8.1093408115643282	10.2987723773365900	F	F	F
3.6086080794409914	7.7809312909323616	8.2518078419286880	F	F	F
2.3009845625244858	6.0539211844920819	11.9218080039603862	F	F	F
5.1211005973608472	4.2802544618489291	14.5050718430130097	F	F	F
3.7262704663302468	6.3487006379506861	12.6701466762358947	F	F	F
1.0890197261047438	6.6356709265700822	16.3075850644738729	T	T	T
4.6628792971827133	6.7285586282620855	17.0313514249285234	T	T	T
6.0530477783191614	5.4393744268118729	15.1474398972362518	T	T	T

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  4.2448350272141049  4.9301833982603611 13.2917821082657603   F   F   F
  1.6036782957222235  8.0064255055192231 15.6115765182596942   T   T   T
  3.5613034081160300  7.4198147397169176 13.8903255655927040   F   F   F
  2.0946400504700109  6.2336711666346920 17.5176660477001320   T   T   T
  2.5694030169158850  8.6156873157450242 20.0668551653921128   T   T   T
  3.5648194419424155  6.3881635800991905 18.1911359170325042   T   T   T
  6.0376313693007981  6.6460321779710485 21.7965028400119003   T   T   T
  5.6568841379258199  5.6585399368278484 20.5746846235569194   T   T   T
  3.8166868494213086  4.9549126082732604 18.9417193648350732   T   T   T
  1.4454566075962552  7.7149417109592058 20.7912166406417533   T   T   T
  3.5889951081569142  7.6290255974758052 19.2575960767526873   T   T   T
  2.0574486274834078  6.1992279723831896 22.8747676006445175   T   T   T
  4.7130472245822679  7.0320007187477387 22.7439303507688422   T   T   T
  3.8835338024535386  5.0100264089964526  7.9999999999999991   F   F   F
  3.6813637476998817  5.9880536531619493  8.0158744918591083   F   F   F
  4.4834445270957994  8.1887145056270061  8.0308754104330902   F   F   F
  0.0607236284725381 -0.3890600634831644 24.4312800796531810   T   T   T
  2.7173694780133215  0.3373221739249720 24.4783924553612202   T   T   T
  8.0037056494746430  1.5553349363803322 24.5565291993618438   T   T   T
  0.6637368042008892  2.2750838607724702 24.4305290553203847   T   T   T
  3.4690727408543953  3.0376291610628861 24.5226075075956516   T   T   T
 -1.1752721573735994  4.2541065282747281 24.5362648791874598   T   T   T
  1.5499418755519605  4.9034906044954942 24.4592397216112367   T   T   T
  4.2996851645423018  5.6345280840511727 24.5242678104750738   T   T   T
 -0.3693624195452383  6.9738590245592862 24.4993742558627545   T   T   T
  2.3390831125466240  7.5828243439208665 24.5125105334828142   T   T   T
  7.9410167324424785  0.1784894104081146 26.7676442960502783   T   T   T
  0.6174504871039899  0.8820857896950988 26.7202466078507328   T   T   T
  6.0141901854459698  2.1937492749193379 26.9209979914146267   T   T   T
 -1.3128120471173641  2.8749296807896680 26.9105872572453251   T   T   T
  1.3808900755488207  3.5274823815150080 26.7118829192469498   T   T   T
 -0.5049589746454417  5.5337072335595385 26.7587393037387606   T   T   T
  2.1569300058231646  6.1980482610398742 26.8802999178715289   T   T   T
  0.2589999319904060  8.2136616109487761 26.7873140912861523   T   T   T
 -4.2157336598196338  8.0925706119914533 29.1360210139122593   T   T   T
 -1.1526898970063806  1.3900577589025966 29.1574018968011863   T   T   T
  1.5130327278945266  2.0883840837134380 29.1107790453893251   T   T   T
  6.9130007547370997  3.4074971798413776 29.2219231712085055   T   T   T
 -0.3673305404856547  4.1007340465013069 29.1485413782385052   T   T   T
  2.3116181261068545  4.7160821292609638 29.1322625903484322   T   T   T
 -2.2924825817202996  6.1085966840965185 29.1768464784889403   T   T   T
  0.3736426447319885  6.7310880338166470 29.1315544026176170   T   T   T
  3.0806916405293321  7.4180073784240328 29.1791350401232172   T   T   T
  6.1448473406096875  0.7309047120440925 29.1689609215738450   T   T   T
  5.4081905888473605  0.9953863573808279 24.4995530022785388   T   T   T
  6.1145646404996068  3.6579560419673709 24.7082943025451343   T   T   T
 -2.9844688580333831  6.2615406507552951 24.6175249536076954   T   T   T
 -2.4079334266851142  7.6108311082420537 26.7905325307187532   T   T   T
  3.3220920814808856  1.5831741812245503 26.8765293627280464   T   T   T
  4.0853534704813672  4.2447170320350329 26.7783760271396716   T   T   T
 -3.1960645531184482  4.9297942804762540 26.9611021114746272   T   T   T
  4.8728617394424933  6.8853874716236998 26.8918102282457276   T   T   T
  3.4619363452173229  0.0831702136555691 29.1668205719924956   T   T   T
  4.2186244426870543  2.7747365397916588 29.1698488089058259   T   T   T
  4.9836776959720339  5.3912554007361049 29.2052375994827074   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Pt E_tot= -884.63881952 eV
 D3-zero damping= -8.9101251 eV, D3-BJ damping= -12.6701745 eV
Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H
O  H Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     9.9890116653035843    0.0000000000000000    0.0000000000000000
    -4.9945058326517895    8.6507378608520060    0.0000000000000000
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     0.0000000000000019    0.0000000000000033   30.8179066174256846
   2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.5755189909298060  0.1847487197400928  9.0169746245084816   F   F   F
 -1.2540702877947054  2.3859442496821237 10.8612336967246357   F   F   F
  2.3103434175182311  2.6365926328492870 11.6081185941916623   F   F   F
  3.5053812231125305  1.4205074907212190  9.5654178022134708   F   F   F
 -0.6310671703315774  3.7839718811383261 10.2987723773365900   F   F   F
  1.1113551631150940  3.4555623605063581  8.2518078419286844   F   F   F
 -0.1962683538014117  1.7285522540660792 11.9218080039603862   F   F   F
  2.6238476810349494 -0.0451144685770741 14.5050718430130097   F   F   F
  1.2290175500043494  2.0233317075246826 12.6701466762358947   F   F   F
 -1.3525835749526509  2.2577223541351459 16.3121249629701772   T   T   T
  2.1792181034880782  2.4852071419003949 16.9728764226471860   T   T   T
  3.5768731815146007  1.0819519498648638 15.1857964309380478   T   T   T
  1.7475821108882081  0.6048144678343575 13.2917821082657603   F   F   F
 -0.8764297637345557  3.6545162009992991 15.6259309515977449   T   T   T
  1.0640504917901330  3.0944458092909142 13.8903255655927005   F   F   F
 -0.3216524584727574  1.8223003080633693 17.4884993135812010   T   T   T
 -0.1568882040697370  4.1127347338831015 19.9756249411432307   T   T   T
  1.1342805817728230  2.1037185026881651 18.1536486332338072   T   T   T
  3.5116237966728097  2.0110454986747563 21.8197827245978040   T   T   T
  2.8894547254346215  0.6144269845492224 21.2590321845126233   T   T   T
  1.5570053706113902  0.7542301853143558 18.9413223507316211   T   T   T
 -1.1617578045289227  2.9773362284078861 20.5515440663527436   T   T   T
  1.0566158558304857  3.3661947442275486 19.1851385045308618   T   T   T
 -0.0746658810664003  1.6280175491806985 22.6019379917011989   T   T   T
  2.4714949585613577  2.7860654510064697 22.8178558031399668   T   T   T
  1.5379264280621523  2.4516985778996228 22.8135741019826099   T   T   T
  0.0034300217279453  0.6712120015727864 22.8169546306788469   T   T   T
  1.3862808861276410  0.6846574785704490  8.0000000000000000   F   F   F
  1.1841108313739839  1.6626847227359456  8.0158744918591047   F   F   F
  1.9861916107699016  3.8633455752010031  8.0308754104330866   F   F   F
  0.0782660746039112  4.5101176501660962  9.0169746245084816   F   F   F
 -3.7513232041206002  6.7113131801081263 10.8612336967246357   F   F   F
 -0.1869094988076636  6.9619615632752900 11.6081185941916623   F   F   F
  1.0081283067866358  5.7458764211472220  9.5654178022134708   F   F   F
 -3.1283200866574723  8.1093408115643300 10.2987723773365900   F   F   F
 -1.3858977532108008  7.7809312909323616  8.2518078419286844   F   F   F
 -2.6935212701273064  6.0539211844920819 11.9218080039603862   F   F   F
  0.1265947647090546  4.2802544618489291 14.5050718430130097   F   F   F
 -1.2682353663215453  6.3487006379506852 12.6701466762358947   F   F   F
 -3.8498364912785457  6.5830912845611484 16.3121249629701772   T   T   T
 -0.3180348128378164  6.8105760723263975 16.9728764226471860   T   T   T
  1.0796202651887057  5.4073208802908672 15.1857964309380478   T   T   T
 -0.7496708054376866  4.9301833982603602 13.2917821082657603   F   F   F
 -3.3736826800604502  7.9798851314253012 15.6259309515977449   T   T   T
 -1.4332024245357617  7.4198147397169176 13.8903255655927005   F   F   F
 -2.8189053747986521  6.1476692384893727 17.4884993135812010   T   T   T
 -2.6541411203956313  8.4381036643091036 19.9756249411432307   T   T   T
 -1.3629723345530718  6.4290874331141685 18.1536486332338072   T   T   T
  1.0143708803469147  6.3364144291007589 21.8197827245978040   T   T   T
  0.3922018091087267  4.9397959292609395 21.2590321845126233   T   T   T
 -0.9402475457145044  5.0795991157403586 18.9413223507316211   T   T   T
 -3.6590107208548175  7.3027051588338887 20.5515440663527436   T   T   T
 -1.4406370604954091  7.6915636746535521 19.1851385045308618   T   T   T
 -2.5719187973922950  5.9533864796067011 22.6019379774154814   T   T   T
 -0.0257579577645369  7.1114343814324732 22.8178558174256807   T   T   T
 -0.9593264882637423  6.7770675083256258 22.8135741019826099   T   T   T
 -2.4938228945979497  4.9965809319987899 22.8169546306788469   T   T   T
 -1.1109720301982537  5.0100264089964517  8.0000000000000000   F   F   F
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-1.3131420849519109	5.9880536531619484	8.0158744918591047	F	F	F
-0.5110613055559932	8.1887145056270061	8.0308754104330866	F	F	F
7.5700248235815977	0.1847487197400928	9.0169746245084816	F	F	F
3.7404355448570867	2.3859442496821237	10.8612336967246357	F	F	F
7.3048492501700233	2.6365926328492870	11.6081185941916623	F	F	F
8.4998870557643222	1.4205074907212190	9.5654178022134708	F	F	F
4.3634386623202150	3.7839718811383261	10.2987723773365900	F	F	F
6.1058609957668857	3.4555623605063581	8.2518078419286844	F	F	F
4.7982374788503801	1.7285522540660792	11.9218080039603862	F	F	F
7.6183535136867420	-0.0451144685770741	14.5050718430130097	F	F	F
6.2235233826561416	2.0233317075246826	12.6701466762358947	F	F	F
3.6419222576991412	2.2577223541351459	16.3121249629701772	T	T	T
7.1737239504255852	2.4852071419003949	16.9728764226471860	T	T	T
8.5713790141663928	1.0819519498648638	15.1857964309380478	T	T	T
6.7420879435400005	0.6048144678343575	13.2917821082657603	F	F	F
4.1180760689172358	3.6545162009992991	15.6259309515977449	T	T	T
6.0585563244419252	3.0944458092909142	13.8903255655927005	F	F	F
4.6728533741790352	1.8223003080633693	17.4884993135812010	T	T	T
4.8376176285820547	4.1127347338831015	19.9756249411432307	T	T	T
6.1287864144246154	2.1037185026881651	18.1536486332338072	T	T	T
8.5061296293246009	2.0110454986747563	21.8197827245978040	T	T	T
7.8839605580864136	0.6144269988349367	21.2590321845126233	T	T	T
6.5515112032631819	0.7542301853143558	18.9413223507316211	T	T	T
3.8327480281228694	2.9773362284078861	20.5515440663527436	T	T	T
6.0511217027679924	3.3661947442275486	19.1851385045308618	T	T	T
4.9198399515853923	1.6280175491806985	22.6019379774154814	T	T	T
7.4660007912131503	2.7860654510064697	22.8178558031399668	T	T	T
6.5324322607139438	2.4516985778996228	22.8135741019826099	T	T	T
4.9979358543797376	0.6712120015727864	22.8169546306788469	T	T	T
6.3807867187794329	0.6846574785704490	8.0000000000000000	F	F	F
6.1786166640257765	1.6626847227359456	8.0158744918591047	F	F	F
6.9806974434216933	3.8633455752010031	8.0308754104330866	F	F	F
5.0727719072557029	4.5101176501660962	9.0169746245084816	F	F	F
1.2431826285311920	6.7113131801081263	10.8612336967246357	F	F	F
4.8075963338441285	6.9619615632752900	11.6081185941916623	F	F	F
6.0026341394384275	5.7458764211472220	9.5654178022134708	F	F	F
1.8661857459943199	8.1093408115643300	10.2987723773365900	F	F	F
3.6086080794409914	7.7809312909323616	8.2518078419286844	F	F	F
2.3009845625244858	6.0539211844920819	11.9218080039603862	F	F	F
5.1211005973608472	4.2802544618489291	14.5050718430130097	F	F	F
3.7262704663302468	6.3487006379506852	12.6701466762358947	F	F	F
1.1446693413732465	6.5830912845611484	16.3121249629701772	T	T	T
4.6764710198139756	6.8105760723263975	16.9728764226471860	T	T	T
6.0741260978404981	5.4073208802908672	15.1857964309380478	T	T	T
4.2448350272141058	4.9301833982603602	13.2917821082657603	F	F	F
1.6208231525913417	7.9798851314253012	15.6259309515977449	T	T	T
3.5613034081160304	7.4198147397169176	13.8903255655927005	F	F	F
2.1756004578531400	6.1476692384893727	17.4884993135812010	T	T	T
2.3403647122561608	8.4381036643091036	19.9756249411432307	T	T	T
3.6315334980987206	6.4290874331141685	18.1536486332338072	T	T	T
6.0088767129987071	6.3364144291007589	21.8197827245978040	T	T	T
5.3867076417605189	4.9397959149752255	21.2590321845126233	T	T	T
4.0542582869372872	5.0795991157403586	18.9413223507316211	T	T	T
1.3354951117969747	7.3027051588338887	20.5515440663527436	T	T	T
3.5538687864420972	7.6915636746535521	19.1851385045308618	T	T	T
2.4225870352594971	5.9533864796067011	22.6019379917011989	T	T	T
4.9687478748872556	7.1114343814324732	22.8178558031399668	T	T	T
4.0351793443880490	6.7770675083256258	22.8135741019826099	T	T	T
2.5006829380538425	4.9965809319987899	22.8169546306788469	T	T	T
3.8835338024535382	5.0100264089964517	8.0000000000000000	F	F	F
3.6813637476998813	5.9880536531619484	8.0158744918591047	F	F	F
4.4834445270957985	8.1887145056270061	8.0308754104330866	F	F	F

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Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Pt E_tot= -240.88255483 eV
 D3-zero damping= -18.780599 eV, D3-BJ damping= -19.9697358 eV
Pt
 1.0000000000000000
     9.9890116653035843    0.0000000000000000    0.0000000000000000
    -4.9945058326517895    8.6507378608520060    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000279564213513  0.0000258120410618  7.9559237021070865
  2.6888474287097353  0.6663550351833702  7.9620202979308763
  8.0675413725701510  1.9955099191570078  7.9619515761381052
  0.7676023515863249  2.6620139154301947  7.9616553992780332
  3.4571832169316501  3.3281234508104727  7.9588539445227511
 -1.1530295244332325  4.6580121106023258  7.9589164208006249
  1.5371529358889420  5.3231630545975248  7.9588858001588703
  4.2270896588724458  5.9889787125569613  7.9620225967944309
 -0.3840403495666888  7.3203106606580306  7.9588313574772185
  2.3053592617877552  7.9844259803839854  7.9616574602269869
  8.4518077323460421  0.4424572025929865 10.2746057103914925
  1.1517583976965742  1.1101005908723622 10.2746798922843361
  6.5294730267516643  2.4377975943684724 10.2743179697971225
 -0.7665599506301107  3.1041907414640462 10.2746937791548802
  1.9216511216143324  3.7737290516687692 10.2752590633296546
 -0.0000479267077819  5.7671047120359100 10.2740485134170605
  2.6895762433108441  6.4347617542009274 10.2747674699649938
  0.7656334006610667  8.4280394972563002 10.2753392473373513
 -3.4580926716978486  8.2073199897837661 12.5884920117861174
 -0.3840655958592716  1.5521435715151155 12.5886101420245815
  2.3050234796748876  2.2177775072667996 12.5909959052532106
  7.6842886680052711  3.5482967658169491 12.5880064701198453
  0.3841665325690535  4.2152242451033359 12.5897887498084522
  3.0740311854048579  4.8804778124865109 12.5880552014686540
 -1.5359153385599909  6.2105146633861867 12.5897050364218845
  1.1520642545678077  6.8755927895948998 12.5897594807205628
  3.8424848917805030  7.5419397916380140 12.5884751474109038
  6.9161063046934892  0.8872121813866373 12.5909595053725845
  5.3781616633969618  1.3299539008279033  7.9588607629560215
  6.1481801115149661  3.9926434531240869  7.9588243871570086
 -3.0728811872080013  6.6549258976832428  7.9616217512498686
 -1.9228654333503150  7.7625527748589018 10.2746765707945755
  3.8409713191906132  1.7772130452956330 10.2743356954962568
  4.6131346416870063  4.4357311543804574 10.2743114546314498
 -2.6871753707183905  5.0997275277775973 10.2753096920567426
  5.3799728841894261  7.0982272614233155 10.2746651989841098
  4.2253841017537681  0.2218936880382691 12.5880773695965278
  4.9946181416426869  2.8835659406919740 12.5882148823768603
  5.7627399792126406  5.5457263301146869 12.5909605692330508

Interface: O-a-SiO2(0001)/fcc(111)_sqrt13/Pd E_tot= -1054.86044986 eV
 D3-zero damping= -26.3240953 eV, D3-BJ damping= -33.4026279 eV
Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O
Si  O  H Pd
 1.0000000000000000
     9.9079872356281502    0.0000000000000000    0.0000000000000000
    -4.9539936178140724    8.5805686464259345    0.0000000000000000
     0.0000000000000023    0.0000000000000039   37.0953567580144039
   2   5   3   6   3   7   2   2   5   3   6   3   7   2   2   5   3   6
3   7   2   2   5   3   6   3   7   2  39
Selective dynamics
Cartesian
  2.5546280395173477  0.1832501571042915  9.0169746245084816   F   F   F
 -1.2438980772451458  2.3665910064839637 10.8612336967246357   F   F   F
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2.2916033995834217	2.6152062913851863	11.6081185941916658	F	F	F
3.4769478281066752	1.4089852487675780	9.5654178022134708	F	F	F
-0.6259483598550004	3.7532787381277863	10.2987723773365900	F	F	F
1.1023405657479666	3.4275330640304671	8.2518078419286880	F	F	F
-0.1946763513127838	1.7145313513739373	11.9218080039603862	F	F	F
2.6025647184121796	-0.0447485290618301	14.5050718430130097	F	F	F
1.2190485511297069	2.0069197437449375	12.6701466762358947	F	F	F
-1.3310350102781459	2.2366585368418206	16.3302200169839331	T	T	T
2.1712148161680438	2.4317988826862313	16.9831820657015022	T	T	T
3.5691690484665100	1.0777816969326219	15.1676471212267838	T	T	T
1.7334068502528102	0.5999086023736188	13.2917821082657603	F	F	F
-0.8502303362943953	3.6269802244468661	15.6436847849685599	T	T	T
1.0554195994524433	3.0693456577183396	13.8903255655927040	F	F	F
-0.3147298443439357	1.7383013402731324	17.5000435272857402	T	T	T
-0.0716360352088246	4.1008098244143891	19.8666809670573947	T	T	T
1.1572744081461201	1.9537694845332843	18.1582366254662446	T	T	T
4.1074200300372476	1.9757146919953541	21.7765229768878008	T	T	T
3.6426119217819926	1.0668675647890000	20.5163922886948988	T	T	T
1.6353435483227092	0.5598275325513956	18.8480947485448276	T	T	T
-1.2527337914477301	3.2219158175741178	20.5612735667460811	T	T	T
1.0903336017357594	3.1159783335865661	19.2973371442899300	T	T	T
0.2970608485577050	2.0423714244679436	22.4448753177927074	T	T	T
2.8955018395095160	1.9295857893766886	22.9128218455022648	T	T	T
1.3750362683484270	0.6791039780257577	8.0000000000000000	F	F	F
1.1745060868808093	1.6491980950390659	8.0158744918591083	F	F	F
1.9700809035366977	3.8320086039011239	8.0308754104330902	F	F	F
0.0776312306103113	4.4735344803172588	9.0169746245084816	F	F	F
-3.7208948861521818	6.6568753296969314	10.8612336967246357	F	F	F
-0.1853934093236145	6.9054906145981541	11.6081185941916658	F	F	F
0.9999510191996390	5.6992695719805448	9.5654178022134708	F	F	F
-3.1029451687620364	8.0435630613407518	10.2987723773365900	F	F	F
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-2.6716731602198203	6.0048156745869044	11.9218080039603862	F	F	F
0.1255679095051436	4.2455357941511371	14.5050718430130097	F	F	F
-1.2579482577773293	6.2972040669579048	12.6701466762358947	F	F	F
-3.8724090909062707	6.5365793748089338	16.3217305647331443	T	T	T
-0.4365486370407047	6.8716699871255322	16.9035323521291261	T	T	T
1.0519384831136791	5.3911488335592805	15.2025944647920781	T	T	T
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-3.3630687118614118	7.9322867015665093	15.6450008134633407	T	T	T
-1.4215772094545929	7.3596299809313068	13.8903255655927040	F	F	F
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-2.3492517585815431	8.5137517822078337	20.0037245280917588	T	T	T
-1.3820324306403302	6.2865336330949688	18.0962007872688382	T	T	T
0.8097328462014800	6.4673974005705910	21.7580908029855209	T	T	T
0.5874750727425444	5.0696482374298917	20.9747726282794602	T	T	T
-0.7563106444566375	4.8919785697846869	18.6293182495069090	T	T	T
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-0.5234792412849328	7.0203608395586086	22.5080407356943901	T	T	T
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-0.5069159053703383	8.1222929271140902	8.0308754104330902	F	F	F
7.5086216573314220	0.1832501571042915	9.0169746245084816	F	F	F
3.7100955405689291	2.3665910064839637	10.8612336967246357	F	F	F
7.2455970173974968	2.6152062913851863	11.6081185941916658	F	F	F
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4.3280452579590749	3.7532787381277863	10.2987723773365900	F	F	F
6.0563341835620417	3.4275330640304671	8.2518078419286880	F	F	F
4.7593172665012915	1.7145313513739373	11.9218080039603862	F	F	F
7.5565583362262547	-0.0447485290618301	14.5050718430130097	F	F	F
6.1730421689437813	2.0069197437449375	12.6701466762358947	F	F	F

3.6381394502737194	2.2195282069889379	16.3264687257367349	T	T	T
7.1201321557304489	2.5307592630988136	16.9730377271081636	T	T	T
8.5091214129210453	1.0794424376915084	15.1858116802398389	T	T	T
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4.1019950764029920	3.6282229926749556	15.6540390922227335	T	T	T
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4.8817790984753779	4.3529622805437045	19.9746391533000818	T	T	T
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8.1578663508728049	0.7666474404649242	21.2674647924901272	T	T	T
6.6731187225545749	0.8872926458205870	19.0045525163614535	T	T	T
4.2277367298922961	3.5170439051148419	21.2167990120757075	T	T	T
5.9186640121770395	3.4052106233168598	19.1687035530318575	T	T	T
5.4777334815990413	1.4458644727201175	22.4795324538720998	T	T	T
7.7900620854650278	2.8949841188342140	23.0407916929027401	T	T	T
6.3290298861625018	0.6791039780257577	8.0000000000000000	F	F	F
6.1284997046948835	1.6491980950390659	8.0158744918591083	F	F	F
6.9240745213507733	3.8320086039011239	8.0308754104330902	F	F	F
5.0316248484243866	4.4735344803172588	9.0169746245084816	F	F	F
1.2330987316618929	6.6568753296969314	10.8612336967246357	F	F	F
4.7686002084904597	6.9054906145981541	11.6081185941916658	F	F	F
5.9539446370137146	5.6992695719805448	9.5654178022134708	F	F	F
1.8510484490520385	8.0435630613407518	10.2987723773365900	F	F	F
3.5793373746550055	7.7178173872434339	8.2518078419286880	F	F	F
2.2823204575942548	6.0048156745869044	11.9218080039603862	F	F	F
5.0795615273192185	4.2455357941511371	14.5050718430130097	F	F	F
3.6960453600367456	6.2972040669579048	12.6701466762358947	F	F	F
1.0523289174415758	6.5892408238223119	16.3110565538383270	T	T	T
4.5640315421969486	6.7121142949761454	16.9926118388580107	T	T	T
6.0132296954697599	5.3976898806007449	15.1583235914284042	T	T	T
4.2104036591598488	4.8901929255865859	13.2917821082657603	F	F	F
1.5766610361037330	7.9583595516323307	15.6190120138055750	T	T	T
3.5324164083594818	7.3596299809313068	13.8903255655927040	F	F	F
2.0239970973585582	6.2092661914441445	17.5529951663619954	T	T	T
2.4744804189346317	8.5178676959246804	20.0720015031329666	T	T	T
3.5084059857364371	6.3695556257929695	18.1898714935495640	T	T	T
6.0103495373334352	6.5843035937813292	21.8220838817742511	T	T	T
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3.8520330772554661	4.9693883012387250	8.0000000000000000	F	F	F
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4.4470777124437362	8.1222929271140902	8.0308754104330902	F	F	F
0.0892729365572274	-0.3595477987914693	24.4066660364557144	T	T	T
2.7278159472692081	0.3749933549634498	24.4238815205763942	T	T	T
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0.6928680765811516	2.2957973242159060	24.3849685922939479	T	T	T
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1.5773334660554250	4.8969147715235488	24.4491158188086288	T	T	T
4.3013694696788969	5.6315836575461118	24.4266292731410637	T	T	T
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8.3075071632710511	0.0857598766345392	26.6942111505019959	T	T	T
1.0533740945096837	0.7858473409262240	26.6574341868951450	T	T	T
6.4054015191289215	2.1177009549235590	26.7936408430593858	T	T	T
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  2.5941715256474986  6.0479932655643482 26.7434008071638694   T   T   T
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  3.6987721112390668  7.1714108093729818 29.0147773646944529   T   T   T
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Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Pd E_tot= -884.85859412 eV
 D3-zero damping= -9.070464 eV, D3-BJ damping= -12.8932967 eV
Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H
O  H Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     9.9079872356281502    0.0000000000000000    0.0000000000000000
    -4.9539936178140724    8.5805686464259345    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.8463929208147860
   2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.5546280395173477  0.1832501571042915  9.0169746245084816   F   F   F
 -1.2438980772451458  2.3665910064839637 10.8612336967246357   F   F   F
  2.2916033995834217  2.6152062913851863 11.6081185941916623   F   F   F
  3.4769478281066752  1.4089852487675780  9.5654178022134708   F   F   F
 -0.6259483598550004  3.7532787381277863 10.2987723773365900   F   F   F
  1.1023405657479666  3.4275330640304671  8.2518078419286844   F   F   F
 -0.1946763513127838  1.7145313513739373 11.9218080039603862   F   F   F
  2.6025647184121796 -0.0447485290618301 14.5050718430130097   F   F   F
  1.2190485511297069  2.0069197437449375 12.6701466762358947   F   F   F
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 -0.8752137261457862  3.6415103934444515 15.6388392522637734   T   T   T
  1.0554195994524433  3.0693456577183396 13.8903255655927005   F   F   F
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  1.1088522964021417  2.0882364426130957 18.1679250127245844   T   T   T
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 -1.1614127727125438  2.9127154759580685 20.5501112179671743   T   T   T
  1.0611511691960751  3.3461645809607101 19.2065837817299290   T   T   T
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  1.5144167213448014  2.4456370113190666 22.8463929208147825   T   T   T
  0.0058547716237236  0.6283435460026778 22.8212964503534508   T   T   T
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0.1255679095051434	4.2455357941511371	14.5050718430130097	F	F	F
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-0.7435899586542261	4.8901929255865859	13.2917821082657603	F	F	F
-3.3522105350528224	7.9317947166574188	15.6388392522637734	T	T	T
-1.4215772094545929	7.3596299809313068	13.8903255655927005	F	F	F
-2.8350423231067183	6.1059657798577831	17.5244083240022483	T	T	T
-2.6448632662398057	8.3579812099674342	19.9953300805837806	T	T	T
-1.3681445125048945	6.3785207658260630	18.1679250127245844	T	T	T
0.9946554019188723	6.2718207683950782	21.8442215909559927	T	T	T
0.3483406626760432	4.8785151674692200	21.3032207774604849	T	T	T
-0.9456061091170480	5.0292351342746988	18.9539277639564006	T	T	T
-3.6384095816195803	7.2029997991710353	20.5501112179671743	T	T	T
-1.4158456397109611	7.6364489041736778	19.2065837817299290	T	T	T
-2.5569722413508189	5.8816559222472531	22.6300457180164294	T	T	T
-0.0317827779900890	7.0795354565441659	22.8325602599548674	T	T	T
-0.9625800875622348	6.7359213345320335	22.8463929208147825	T	T	T
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-1.3024907220262270	5.9394824182520329	8.0158744918591047	F	F	F
-0.5069159053703385	8.1222929271140920	8.0308754104330866	F	F	F
7.5086216573314228	0.1832501571042915	9.0169746245084816	F	F	F
3.7100955405689291	2.3665910064839637	10.8612336967246357	F	F	F
7.2455970173974968	2.6152062913851863	11.6081185941916623	F	F	F
8.4309414459207499	1.4089852487675780	9.5654178022134708	F	F	F
4.3280452579590749	3.7532787381277863	10.2987723773365900	F	F	F
6.0563341835620417	3.4275330640304671	8.2518078419286844	F	F	F
4.7593172665012915	1.7145313513739373	11.9218080039603862	F	F	F
7.5565583362262547	-0.0447485290618301	14.5050718430130097	F	F	F
6.1730421689437822	2.0069197437449375	12.6701466762358947	F	F	F
3.5959990668598940	2.2460518131524352	16.3202770808409845	T	T	T
7.0766871935828490	2.4649566017638902	16.9590122000833361	T	T	T
8.5143804312553044	1.0797436136709435	15.1843282764758847	T	T	T
6.6874004680668850	0.5999086023736188	13.2917821082657603	F	F	F
4.0787798916682885	3.6415103934444515	15.6388392522637734	T	T	T
6.0094132172665180	3.0693456577183396	13.8903255655927005	F	F	F
4.5959481036143934	1.8156814566448161	17.5244083240022483	T	T	T
4.7861271604813060	4.0676968867544669	19.9953300805837806	T	T	T
6.0628459142162168	2.0882364426130957	18.1679250127245844	T	T	T
8.4256458286399827	1.9815364451821109	21.8442215909559927	T	T	T
7.7793310893971546	0.5882308442562524	21.3032207774604849	T	T	T
6.4853843176040638	0.7389508110617314	18.9539277639564006	T	T	T
3.7925808451015310	2.9127154759580685	20.5501112179671743	T	T	T
6.0151447870101507	3.3461645809607101	19.2065837817299290	T	T	T
4.8740181853702929	1.5913715990342858	22.6300457180164294	T	T	T
7.3992076487310223	2.7892511333311987	22.8325602599548674	T	T	T
6.4684103391588765	2.4456370113190666	22.8463929208147825	T	T	T
4.9598483894377985	0.6283435460026778	22.8212964503534508	T	T	T
6.3290298861625018	0.6791039780257577	8.0000000000000000	F	F	F
6.1284997046948844	1.6491980950390659	8.0158744918591047	F	F	F
6.9240745213507733	3.8320086039011239	8.0308754104330866	F	F	F

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  5.0316248484243866  4.4735344803172588  9.0169746245084816   F   F   F
  1.2330987316618931  6.6568753296969305 10.8612336967246357   F   F   F
  4.7686002084904606  6.9054906145981541 11.6081185941916623   F   F   F
  5.9539446370137146  5.6992695719805457  9.5654178022134708   F   F   F
  1.8510484490520385  8.0435630613407536 10.2987723773365900   F   F   F
  3.5793373746550055  7.7178173872434339  8.2518078419286844   F   F   F
  2.2823204575942553  6.0048156745869044 11.9218080039603862   F   F   F
  5.0795615273192185  4.2455357941511371 14.5050718430130097   F   F   F
  3.6960453600367460  6.2972040669579048 12.6701466762358947   F   F   F
  1.1190022579528578  6.5363361363654029 16.3202770808409845   T   T   T
  4.5996903846758119  6.7552409249768575 16.9590122000833361   T   T   T
  6.0373836223482682  5.3700279368839112 15.1843282764758847   T   T   T
  4.2104036591598488  4.8901929255865859 13.2917821082657603   F   F   F
  1.6017830827612527  7.9317947166574188 15.6388392522637734   T   T   T
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  2.3091303515742694  8.3579812099674342 19.9953300805837806   T   T   T
  3.5858491053091806  6.3785207658260630 18.1679250127245844   T   T   T
  5.9486490197329474  6.2718207683950782 21.8442215909559927   T   T   T
  5.3023342804901183  4.8785151674692200 21.3032207774604849   T   T   T
  4.0083875086970266  5.0292351342746988 18.9539277639564006   T   T   T
  1.3155840361944950  7.2029997991710353 20.5501112179671743   T   T   T
  3.5381479781031140  7.6364489041736778 19.2065837817299290   T   T   T
  2.3970213764632562  5.8816559222472531 22.6300457180164294   T   T   T
  4.9222108398239861  7.0795354565441659 22.8325602599548674   T   T   T
  3.9914135302518403  6.7359213345320335 22.8463929208147825   T   T   T
  2.4828515805307627  4.9186278692156451 22.8212964503534508   T   T   T
  3.8520330772554656  4.9693883012387250  8.0000000000000000   F   F   F
  3.6515028957878481  5.9394824182520329  8.0158744918591047   F   F   F
  4.4470777124437362  8.1222929271140920  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Pd E_tot= -203.29086678 eV
 D3-zero damping= -14.1335784 eV, D3-BJ damping= -17.3791559 eV
Pd
 1.0000000000000000
     9.9079872356281502    0.0000000000000000    0.0000000000000000
    -4.9539936178140724    8.5805686464259345    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000804348190537  0.0000299130449570  7.9936653394070518
  2.6668000938447247  0.6604977463985356  7.9942299257631557
  8.0026839546889441  1.9792427764581855  7.9943194798666006
  0.7614427512627229  2.6397108308667354  7.9943438061797245
  3.4296738642570963  3.3003656400083168  7.9936929530415632
 -1.1433433499832180  4.6202337821079045  7.9944228590358515
  1.5244976003531299  5.2802822959778579  7.9944812978140769
  4.1926882507082093  5.9409111877795953  7.9942527662404528
 -0.3810054367097065  7.2607048967346568  7.9943704577043393
  2.2873628551369474  7.9201988218729946  7.9943367342120988
  8.3835364423602279  0.4401737586667512 10.2753727135905280
  1.1435791498117882  1.1001996280509680 10.2753926178517414
  6.4788180259349959  2.4204384901752465 10.2744204594623039
 -0.7614548468274647  3.0805353940403570 10.2749773481867486
  1.9055838157271734  3.7411733384295842 10.2741560087492445
  0.0000608870106830  5.7203816383873232 10.2745057092182623
  2.6669573279511822  6.3808681341793951 10.2749424590986393
  0.7613719864049624  8.3601965415958688 10.2741104984627025
 -3.4295051277264652  8.1399476438472824 12.5556784252318749
 -0.3808394026955591  1.5404883074634019 12.5557160415399824
  2.2871672760056541  2.1996307654225564 12.5546586921569912
  7.6209922453581687  3.5211696283263425 12.5548285934311981
  0.3818766296834039  4.1800119318989459 12.5549654079051756
```

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  3.0481268888229871  4.8392993651978715 12.5548365581039167
 -1.5248075636021066  6.1598706896419069 12.5549411919367664
  1.1431161321909917  6.8211803096437604 12.5549358917431526
  3.8102448470560017  7.4805330704592539 12.5555670991557111
  6.8594469436506680  0.8809469349482081 12.5547603054472638
  5.3350134128532511  1.3199725251857235  7.9936947853810221
  6.0974106551268896  3.9602099041101719  7.9935851064191459
 -3.0486078564774410  6.6013517036288647  7.9942852582296435
 -1.9053351745000715  7.6997329949379480 10.2749011031753792
  3.8108252833779015  1.7595185996001728 10.2743780357200567
  4.5724412025248053  4.4006444975385310 10.2742775480308808
 -2.6667782949926733  5.0596709526469121 10.2741359449358729
  5.3351086132304140  7.0401873165473106 10.2753635192184714
  4.1929685941927293  0.2200380022237894 12.5546762947466579
  4.9540485088940303  2.8601491493486293 12.5562440057503277
  5.7153651913864687  5.4998473058185322 12.5547132063225444

Interface: O-a-SiO2(0001)/fcc(111)_sqrt13/Ir E_tot= -1192.9028344 eV
 D3-zero damping= -29.6514433 eV, D3-BJ damping= -35.2147549 eV
Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O
Si  O  H Ir
 1.0000000000000000
     9.7892996361861151    0.0000000000000000    0.0000000000000000
    -4.8946498180930549    8.4777821701949385    0.0000000000000000
     0.0000000000000023    0.0000000000000039   37.0752466640440019
   2   5   3   6   3   7   2   2   5   3   6   3   7   2   2   5   3   6
3   7   2   2   5   3   6   3   7   2  39
Selective dynamics
Cartesian
  2.5240261965529829  0.1810550067950667  9.0169746245084816   F   F   F
 -1.2289974447324286  2.3382416557287815 10.8612336967246357   F   F   F
  2.2641523240116115  2.5838787826401126 11.6081185941916658   F   F   F
  3.4352975331184812  1.3921070400205859  9.5654178022134708   F   F   F
 -0.6184501358021149  3.7083182801789341 10.2987723773365900   F   F   F
  1.0891356480987255  3.3864747076051431  8.2518078419286880   F   F   F
 -0.1923443268303175  1.6939930114040453 11.9218080039603862   F   F   F
  2.5713886428405308 -0.0442124872435874 14.5050718430130097   F   F   F
  1.2044455906397500  1.9828788885244766 12.6701466762358947   F   F   F
 -1.3157825452309120  2.1851660475405543 16.3161007055020093   T   T   T
  2.0587710279176226  2.4382861103528910 16.9700284238290742   T   T   T
  3.5317267685725549  1.0645273312572523 15.2092665736111776   T   T   T
  1.7126424010241026  0.5927223081034447 13.2917821082657603   F   F   F
 -0.8336031747727005  3.5999645061202474 15.6773575793917175   T   T   T
  1.0427767472076763  3.0325780217385043 13.8903255655927040   F   F   F
 -0.3734196459252762  1.6924826625361054 17.5508076394053312   T   T   T
  0.0638037324623122  4.2397669905331057 19.9108178890901826   T   T   T
  1.1020232516541761  1.9408289153715204 18.1863487071783432   T   T   T
  4.1157799680274643  2.1505318945896783 21.8081126065493152   T   T   T
  3.6257564995120726  1.3218648564189115 20.4935089626926654   T   T   T
  1.6309148329380669  0.5721053618654479 18.8861043688412629   T   T   T
 -0.9821709845044667  3.6430238097344172 21.0005529152224213   T   T   T
  1.0373688199185243  3.0780115932971190 19.3446056654357008   T   T   T
  0.3594700223932865  1.9760582353223923 22.6794540071795758   T   T   T
  2.8880433049898628  2.6589667784298161 22.7532756337929953   T   T   T
  1.3585647338223068  0.6709690037866327  8.0000000000000000   F   F   F
  1.1604366997624374  1.6294423809621736  8.0158744918591083   F   F   F
  1.9464813401151226  3.7861050423177183  8.0308754104330902   F   F   F
  0.0767012875064550  4.4199460918925366  9.0169746245084816   F   F   F
 -3.6763223537789562  6.5771327408262508 10.8612336967246357   F   F   F
 -0.1831725850349163  6.8227698677375832 11.6081185941916658   F   F   F
  0.9879726240719533  5.6309981251180554  9.5654178022134708   F   F   F
 -3.0657750448486425  7.9472093652764029 10.2987723773365900   F   F   F
 -1.3581892609478019  7.6253657927026124  8.2518078419286880   F   F   F
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-2.6396692358768457	5.9328840965015148	11.9218080039603862	F	F	F
0.1240637337940033	4.1946785978538816	14.5050718430130097	F	F	F
-1.2428793184067777	6.2217699736219458	12.6701466762358947	F	F	F
-3.8517378425042668	6.4841265529224366	16.3573866556623884	T	T	T
-0.4463863402294535	6.8010335799659707	16.8873676245627671	T	T	T
1.0583144018967752	5.3504145976573456	15.1691131254149365	T	T	T
-0.7346825080224251	4.8316133932009144	13.2917821082657603	F	F	F
-3.3552517951900369	7.8599617925686376	15.6407888794858820	T	T	T
-1.4045481618388513	7.2714691068359745	13.8903255655927040	F	F	F
-2.8580741000915633	6.0771531467536466	17.5766919615329513	T	T	T
-2.2066774461476233	8.5576036396100008	20.0320369012489046	T	T	T
-1.3573273974153726	6.2931313812096894	18.1385493460246252	T	T	T
0.9608502497779533	6.4209252621683168	21.8556802391993763	T	T	T
0.9887435290948385	5.3386043755826806	20.6527594497442983	T	T	T
-0.7894660594045935	4.8770936236578946	18.6899275550197466	T	T	T
-2.9633150740461378	8.0193741797493203	21.3701825070346487	T	T	T
-1.3092214081200562	7.3725060031361398	19.3612221399748066	T	T	T
-3.1221405955513672	5.6624628095581171	22.7801561417440581	T	T	T
-0.4764022047549548	6.5688701036895196	22.6146225242790599	T	T	T
-1.0887601752242209	4.9098600888841029	8.0000000000000000	F	F	F
-1.2868882092840903	5.8683334660596431	8.0158744918591083	F	F	F
-0.5008435689314049	8.0249961274151875	8.0308754104330902	F	F	F
7.4186760146460404	0.1810550067950667	9.0169746245084816	F	F	F
3.6656523733606292	2.3382416557287815	10.8612336967246357	F	F	F
7.1588021421046690	2.5838787826401126	11.6081185941916658	F	F	F
8.3299473512115387	1.3921070400205859	9.5654178022134708	F	F	F
4.2761996822909429	3.7083182801789341	10.2987723773365900	F	F	F
5.9837854661917840	3.3864747076051431	8.2518078419286880	F	F	F
4.7023054912627407	1.6939930114040453	11.9218080039603862	F	F	F
7.4660384609335892	-0.0442124872435874	14.5050718430130097	F	F	F
6.0990954087328078	1.9828788885244766	12.6701466762358947	F	F	F
3.5438824994900568	2.2299566564849869	16.3495270434664164	T	T	T
6.9757463670060513	2.3740418771346228	16.8882453365470582	T	T	T
8.4705814533487480	1.0691319617453889	15.1350503627737663	T	T	T
6.6072922191171601	0.5927223081034447	13.2917821082657603	F	F	F
4.0104384615006055	3.6147515495663693	15.6443332046248429	T	T	T
5.9374265653007345	3.0325780217385043	13.8903255655927040	F	F	F
4.5289716410217178	1.8350171476631345	17.5832805202641076	T	T	T
5.0739600890977492	4.4483807775914599	19.9429523758042144	T	T	T
6.0109544534625643	2.1631469482176726	18.1717725887903754	T	T	T
8.7551831938508027	2.2990865912578187	21.8997759815269930	T	T	T
8.3394694500733006	1.0696200689164070	20.9481489959448481	T	T	T
6.4436820024916521	0.9053190665470621	19.0970343126632223	T	T	T
4.7634811044193093	3.5434475887916324	21.2548972392077147	T	T	T
6.0732732883631613	3.5530375401352283	19.0209224991257777	T	T	T
5.1286652996553421	1.2091819825335561	22.6920823122185347	T	T	T
7.6073873050063057	2.6553201680459297	23.0742863106401046	T	T	T
6.2532145519153648	0.6709690037866327	8.0000000000000000	F	F	F
6.0550865178554947	1.6294423809621736	8.0158744918591083	F	F	F
6.8411311582081806	3.7861050423177183	8.0308754104330902	F	F	F
4.9713511055995134	4.4199460918925366	9.0169746245084816	F	F	F
1.2183274643141015	6.5771327408262508	10.8612336967246357	F	F	F
4.7114772330581411	6.8227698677375832	11.6081185941916658	F	F	F
5.8826224421650117	5.6309981251180554	9.5654178022134708	F	F	F
1.8288747732444153	7.9472093652764029	10.2987723773365900	F	F	F
3.5364605571452561	7.6253657927026124	8.2518078419286880	F	F	F
2.2549805822162128	5.9328840965015148	11.9218080039603862	F	F	F
5.0187135518870614	4.1946785978538816	14.5050718430130097	F	F	F
3.6517704996862803	6.2217699736219458	12.6701466762358947	F	F	F
1.0450387643447727	6.5018602910971817	16.3184088376284286	T	T	T
4.4610876090055145	6.6508338687719242	17.0215602886575645	T	T	T
5.9522465744814310	5.3225016347083720	15.2119319455936335	T	T	T
4.1599673100706323	4.8316133932009144	13.2917821082657603	F	F	F

```
  1.5916116437677248  7.8853272014306084 15.6724204150721249   T   T   T
  3.4901016562542062  7.2714691068359745 13.8903255655927040   F   F   F
  1.9650327778972152  6.0323377500175788 17.5715635286556733   T   T   T
  2.4731969427344698  8.5420122113957468 20.1333048092125750   T   T   T
  3.4308269956866400  6.2627575888349662 18.2308520379381420   T   T   T
  5.9074946188742095  6.7450981699312100 21.8165046832216554   T   T   T
  5.6630171318818290  5.8814584562631875 20.4480791076108197   T   T   T
  3.8051858442400373  4.8649870551680596 18.9927591731196479   T   T   T
  1.5359506367466280  7.7859477380513153 21.2171527285921542   T   T   T
  3.3865926561549480  7.4908350372489654 19.2997397429050110   T   T   T
  2.0242998628144204  5.8614007343798455 23.0341971554155052   T   T   T
  4.5953450550933370  7.3381164704428858 22.6219921229407497   T   T   T
  3.8058896428688374  4.9098600888841029  8.0000000000000000   F   F   F
  3.6077616088089677  5.8683334660596431  8.0158744918591083   F   F   F
  4.3938062491616527  8.0249961274151875  8.0308754104330902   F   F   F
 -0.2098783051434972 -0.6855153397145733 24.5995046645028026   T   T   T
  2.4063722572002066  0.0118183940796598 24.7127248344551091   T   T   T
  7.6677299783315140  1.3239265161466194 24.7229309372379866   T   T   T
  0.5051832498140946  1.9575065764412019 24.6614709550655746   T   T   T
  3.1254830270920486  2.6397596127861016 24.6989797281651775   T   T   T
 -1.3562047740763017  3.8976197894494558 24.7275082713867249   T   T   T
  1.3023795508992144  4.6233790307755616 24.7113044332175278   T   T   T
  3.9244730921874456  5.2125650161515127 24.7623527327590480   T   T   T
 -0.6072401704301813  6.5667007179305124 24.6172402535344332   T   T   T
  2.0573038007806508  7.1742341212970571 24.7073723656951927   T   T   T
  8.0611290800387874 -0.2014633008912126 26.8038801357679297   T   T   T
  0.8795462813968146  0.4574356541571294 26.8179332475789991   T   T   T
  6.1655742742763380  1.7357601650456949 26.8900769269815711   T   T   T
 -0.9746798659776894  2.3998124110208123 26.8978472955517134   T   T   T
  1.6276168872017880  3.0565533328648740 26.8213395592672121   T   T   T
 -0.2360614803440821  5.0335738436487611 26.8096720096247410   T   T   T
  2.3972831670743675  5.6859718924532139 26.9580117016729304   T   T   T
  0.5115681037890097  7.6389208582735728 26.8063719496601678   T   T   T
 -3.6281895473281520  7.4219358551281784 29.0420311079311411   T   T   T
 -0.5922611434715724  0.8803303253001015 29.0408963602981665   T   T   T
  2.0428277428009625  1.5412704561505268 29.0363689869507766   T   T   T
  7.3033445077122439  2.8347275097029163 29.0573175430783124   T   T   T
  0.1422823504936755  3.5025372242299175 29.0314242833273930   T   T   T
  2.7801507437977269  4.1381309814476417 29.0531184853158209   T   T   T
 -1.7245621194859644  5.4668042287806928 29.0323210612382390   T   T   T
  0.8984414846385924  6.1122251226178781 29.0677715773266492   T   T   T
  3.5516552516900037  6.7565093500220490 29.0751736497582876   T   T   T
  6.5484055195781945  0.2257121330524291 29.0268307806602870   T   T   T
  5.0351382314505582  0.7225214163887034 24.6402399665695633   T   T   T
  5.7732122237450385  3.2962779452020072 24.7638978967963013   T   T   T
 -3.2138812988578085  5.8700467739927440 24.7207898184960904   T   T   T
 -2.1008809768449375  6.9751523203655630 26.8384551878555548   T   T   T
  3.5274713397005106  1.1042738810021984 26.8415319907046488   T   T   T
  4.2696669304540364  3.7042613211118240 26.8627319048267772   T   T   T
 -2.8630972294578871  4.3722648192417486 26.9011885367280357   T   T   T
  5.0547930537581305  6.3424698233984804 26.8597500164168927   T   T   T
  3.9218259763183556 -0.4239119976800756 29.0441511304495954   T   T   T
  4.6542374992045055  2.1898440101525241 29.0347622290546212   T   T   T
  5.4274744051954507  4.8095338652557089 29.0463745472039143   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Ir E_tot= -884.43308581 eV
 D3-zero damping= -9.3032294 eV, D3-BJ damping= -13.2208744 eV
Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H
O  H Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     9.7892996361861151    0.0000000000000000    0.0000000000000000
    -4.8946498180930549    8.4777821701949385    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.8948363045544667
```

```
   2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.5240261965529829  0.1810550067950667  9.0169746245084816   F   F   F
 -1.2289974447324286  2.3382416557287815 10.8612336967246357   F   F   F
  2.2641523240116115  2.5838787826401126 11.6081185941916623   F   F   F
  3.4352975331184812  1.3921070400205859  9.5654178022134708   F   F   F
 -0.6184501358021149  3.7083182801789341 10.2987723773365900   F   F   F
  1.0891356480987255  3.3864747076051431  8.2518078419286844   F   F   F
 -0.1923443268303175  1.6939930114040453 11.9218080039603862   F   F   F
  2.5713886428405308 -0.0442124872435874 14.5050718430130097   F   F   F
  1.2044455906397500  1.9828788885244766 12.6701466762358947   F   F   F
 -1.3675305268674771  2.2291341710531745 16.3313637095106934   T   T   T
  2.0413192601522603  2.4318543570202995 16.9463885587382030   T   T   T
  3.5332192350643976  1.0809167081442406 15.1787914748821784   T   T   T
  1.7126424010241026  0.5927223081034447 13.2917821082657603   F   F   F
 -0.8749368337455341  3.6236599847793833 15.6578476775341944   T   T   T
  1.0427767472076763  3.0325780217385043 13.8903255655927005   F   F   F
 -0.4104770919131119  1.7985986546693886 17.5688040916799473   T   T   T
 -0.1918585417673155  3.9997787437674157 20.0288750722412239   T   T   T
  1.0668977562232216  2.0610882077959176 18.1899592163093047   T   T   T
  3.4027849873652460  1.9381174567353259 21.8871259229484778   T   T   T
  2.7302014238166059  0.5485974691462773 21.3677629095749353   T   T   T
  1.4811687361428545  0.7135520622332823 18.9794298196558202   T   T   T
 -1.1686836891903691  2.8202412079661441 20.5600279991444808   T   T   T
  1.0541776608882734  3.3127672574335558 19.2370943110514858   T   T   T
 -0.1007728408711339  1.5466760653477982 22.6869135916803977   T   T   T
  2.3924505342331481  2.7853534245943661 22.8611502136323388   T   T   T
  1.4627066227425092  2.4375534674581969 22.8948384045544628   T   T   T
 -0.0071182170261494  0.5782292102817279 22.8590834708291837   T   T   T
  1.3585647338223068  0.6709690037866327  8.0000000000000000   F   F   F
  1.1604366997624374  1.6294423809621736  8.0158744918591047   F   F   F
  1.9464813401151226  3.7861050423177183  8.0308754104330866   F   F   F
  0.0767012875064554  4.4199460918925357  9.0169746245084816   F   F   F
 -3.6763223537789562  6.5771327408262508 10.8612336967246357   F   F   F
 -0.1831725850349160  6.8227698677375823 11.6081185941916623   F   F   F
  0.9879726240719537  5.6309981251180554  9.5654178022134708   F   F   F
 -3.0657750448486425  7.9472093652764038 10.2987723773365900   F   F   F
 -1.3581892609478019  7.6253657927026124  8.2518078419286844   F   F   F
 -2.6396692358768448  5.9328840965015148 11.9218080039603862   F   F   F
  0.1240637337940034  4.1946785978538816 14.5050718430130097   F   F   F
 -1.2428793184067775  6.2217699736219458 12.6701466762358947   F   F   F
 -3.8148554359140046  6.4680252561506437 16.3313637095106934   T   T   T
 -0.4060056488942672  6.6707454421177692 16.9463885587382030   T   T   T
  1.0858943260178699  5.3198077932417096 15.1787914748821784   T   T   T
 -0.7346825080224249  4.8316133932009144 13.2917821082657603   F   F   F
 -3.3222617427920618  7.8625510698768517 15.6578476775341944   T   T   T
 -1.4045481618388511  7.2714691068359736 13.8903255655927005   F   F   F
 -2.8578020009596394  6.0374897397668583 17.5688040916799473   T   T   T
 -2.6391834508138432  8.2386698288648859 20.0288750722412239   T   T   T
 -1.3804271528233059  6.2999792928933873 18.1899592163093047   T   T   T
  0.9554600783187185  6.1770085418327954 21.8871259086627639   T   T   T
  0.2828765147700786  4.7874885542437466 21.3677629095749353   T   T   T
 -0.9661561729036731  4.9524431473307517 18.9794298196558202   T   T   T
 -3.6160085982368968  7.0591322930636133 20.5600279991444808   T   T   T
 -1.3931472481582541  7.5516583425310255 19.2370943110514858   T   T   T
 -2.5480977499176616  5.7855671504452681 22.6869135916803977   T   T   T
 -0.0548743748133795  7.0242445096918349 22.8611502136323388   T   T   T
 -0.9846182863040182  6.6764445525556662 22.8948384045544628   T   T   T
 -2.4544431260726771  4.8171202953791967 22.8590834708291837   T   T   T
 -1.0887601752242206  4.9098600888841020  8.0000000000000000   F   F   F
 -1.2868882092840901  5.8683334660596431  8.0158744918591047   F   F   F
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-0.5008435689314048	8.0249961274151875	8.0308754104330866	F	F	F
7.4186760146460404	0.1810550067950667	9.0169746245084816	F	F	F
3.6656523733606292	2.3382416557287815	10.8612336967246357	F	F	F
7.1588021421046690	2.5838787826401126	11.6081185941916623	F	F	F
8.3299473512115387	1.3921070400205859	9.5654178022134708	F	F	F
4.2761996822909429	3.7083182801789341	10.2987723773365900	F	F	F
5.9837854661917831	3.3864747076051431	8.2518078419286844	F	F	F
4.7023054912627398	1.6939930114040453	11.9218080039603862	F	F	F
7.4660384609335884	-0.0442124872435874	14.5050718430130097	F	F	F
6.0990954087328078	1.9828788885244766	12.6701466762358947	F	F	F
3.5271192912255804	2.2291341710531745	16.3313637095106934	T	T	T
6.9359690782453178	2.4318543570202995	16.9463885730239205	T	T	T
8.4278690531574547	1.0809167081442406	15.1787914748821784	T	T	T
6.6072922191171601	0.5927223081034447	13.2917821082657603	F	F	F
4.0197129843475237	3.6236599847793833	15.6578476775341944	T	T	T
5.9374265653007336	3.0325780217385043	13.8903255655927005	F	F	F
4.4841727261799456	1.7985986546693886	17.5688040916799473	T	T	T
4.7027912763257422	3.9997787437674157	20.0288750722412239	T	T	T
5.9615475743162794	2.0610882077959176	18.1899592163093047	T	T	T
8.2974348054583036	1.9381174567353259	21.8871259229484778	T	T	T
7.6248512419096635	0.5485974691462773	21.3677629095749353	T	T	T
6.3758185542359120	0.7135520622332823	18.9794298196558202	T	T	T
3.7259661289026882	2.8202412079661441	20.5600279991444808	T	T	T
5.9488274789813307	3.3127672574335558	19.2370943110514858	T	T	T
4.7938769772219239	1.5466760653477982	22.6869135916803977	T	T	T
7.2871003523262052	2.7853534245943661	22.8611502136323388	T	T	T
6.3573564408355665	2.4375534674581969	22.8948384045544628	T	T	T
4.8875316010669083	0.5782292102817279	22.8590834708291837	T	T	T
6.2532145519153648	0.6709690037866327	8.0000000000000000	F	F	F
6.0550865178554947	1.6294423809621736	8.0158744918591047	F	F	F
6.8411311582081797	3.7861050423177183	8.0308754104330866	F	F	F
4.9713511055995134	4.4199460918925357	9.0169746245084816	F	F	F
1.2183274643141015	6.5771327408262508	10.8612336967246357	F	F	F
4.7114772330581420	6.8227698677375823	11.6081185941916623	F	F	F
5.8826224421650117	5.6309981251180554	9.5654178022134708	F	F	F
1.8288747732444151	7.9472093652764038	10.2987723773365900	F	F	F
3.5364605571452556	7.6253657927026124	8.2518078419286844	F	F	F
2.2549805822162128	5.9328840965015148	11.9218080039603862	F	F	F
5.0187135518870605	4.1946785978538816	14.5050718430130097	F	F	F
3.6517704996862799	6.2217699736219458	12.6701466762358947	F	F	F
1.0797943821790530	6.4680252561506437	16.3313637095106934	T	T	T
4.4886441691987908	6.6707454421177692	16.9463885730239205	T	T	T
5.9805441441109277	5.3198077932417096	15.1787914748821784	T	T	T
4.1599673100706323	4.8316133932009144	13.2917821082657603	F	F	F
1.5723880753009960	7.8625510698768517	15.6578476775341944	T	T	T
3.4901016562542067	7.2714691068359736	13.8903255655927005	F	F	F
2.0368478171334181	6.0374897540525723	17.5688040916799473	T	T	T
2.2554663672792143	8.2386698288648859	20.0288750722412239	T	T	T
3.5142226652697519	6.2999792928933873	18.1899592163093047	T	T	T
5.8501098964117757	6.1770085418327954	21.8871259086627639	T	T	T
5.1775263328631365	4.7874885542437466	21.3677629095749353	T	T	T
3.9284936309036702	4.9524431473307517	18.9794298196558202	T	T	T
1.2786412341418751	7.0591322930636133	20.5600279991444808	T	T	T
3.5015025556490893	7.5516583425310255	19.2370943110514858	T	T	T
2.3465520681753960	5.7855671504452681	22.6869135916803977	T	T	T
4.8397754432796773	7.0242445096918349	22.8611502136323388	T	T	T
3.9100315317890395	6.6764445525556662	22.8948384045544628	T	T	T
2.4402066920203804	4.8171202953791967	22.8590834708291837	T	T	T
3.8058896428688369	4.9098600888841020	8.0000000000000000	F	F	F
3.6077616088089677	5.8683334660596431	8.0158744918591047	F	F	F
4.3938062491616527	8.0249961274151875	8.0308754104330866	F	F	F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Ir E_tot= -338.60687474 eV

```
 D3-zero damping= -17.3430281 eV, D3-BJ damping= -18.8938231 eV
Ir
 1.0000000000000000
     9.7892996361861151    0.0000000000000000    0.0000000000000000
    -4.8946498180930549    8.4777821701949385    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000339838607237  0.0000149689493741  8.1022092024089538
  2.6354221359004910  0.6522360181626565  8.1012089165750449
  7.9067901601629069  1.9562165936200098  8.1012418181822792
  0.7529855489465405  2.6085435658787981  8.1013251254128651
  3.3886170685453898  3.2606294367178346  8.1007597948498198
 -1.1293978350082048  4.5648055375861674  8.1013777841543479
  1.5061491412019270  5.2173121997853817  8.1013979028178689
  4.1418212141843798  5.8693755731893873  8.1012353840134121
 -0.3766666991144472  7.1735053313813770  8.1013689757231298
  2.2591662025786539  7.8256402630238524  8.1013215467351944
  8.2832841574688612  0.4352443942661725 10.2751948556196577
  1.1300527952782971  1.0866588531537928 10.2751621351987161
  6.4007639914355732  2.3911004439254016 10.2743682422214011
 -0.7530095655332623  3.0435982281693645 10.2744233115862045
  1.8825703157316118  3.6953834289035594 10.2746941107823115
  0.0000401411746834  5.6518516112484134 10.2745237901068602
  2.6353922177309168  6.3038301063250017 10.2744336408766728
  0.7531236719969402  8.2604041827730370 10.2746829026872177
 -3.3885974866468809  8.0422751971075268 12.4482991716437734
 -0.3757694716661100  1.5219705122372462 12.4482958971987454
  2.2596706474058936  2.1735532731296590 12.4481390381976880
  7.5305559405516798  3.4781726711039975 12.4478073995758756
  0.3769846091451847  4.1302885136182095 12.4478682636697151
  3.0119113794394718  4.7824898793033883 12.4478131369400220
 -1.5060920836187310  6.0861729046250836 12.4478750938555454
  1.1293052745269108  6.7390077533098971 12.4478603527519311
  3.7645672717533039  7.3912918629067166 12.4483106195874722
  6.7771903158020130  0.8700514738007019 12.4481745287637136
  5.2712528847385531  1.3043153931106848  8.1007521853615909
  6.0241356747397816  3.9128533610989185  8.1007756569137630
 -3.0120500298796626  6.5214322682412105  8.1013079220898891
 -1.8822443272911806  7.6081252946450979 10.2744132659560261
  3.7651002692881335  1.7389940810990501 10.2743334628870908
  4.5181892219417596  4.3476251827669934 10.2743650313614285
 -2.6355792765824653  4.9997372597502272 10.2746973856614900
  5.2707419809848108  6.9558553464760751 10.2751686235465076
  4.1416660126175184  0.2170460005446599 12.4477935700548290
  4.8947039763361309  2.8258896062873697 12.4480040985242102
  5.6472782643916135  5.4341081583626867 12.4481521140061169

Interface: O-a-SiO2(0001)/fcc(111)_sqrt13/Rh E_tot= -1130.26370122 eV
 D3-zero damping= -26.5093339 eV, D3-BJ damping= -33.5753325 eV
Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O
Si  O  H Rh
 1.0000000000000000
     9.6544501462291485    0.0000000000000000    0.0000000000000000
    -4.8272250731145716    8.3609990862048331    0.0000000000000000
     0.0000000000000023    0.0000000000000039   36.9888032229158199
   2   5   3   6   3   7   2   2   5   3   6   3   7   2   2   5   3   6
3   7   2   2   5   3   6   3   7   2  39
Selective dynamics
Cartesian
  2.4892572490396141  0.1785609391673665  9.0169746245084834   F   F   F
 -1.2120677679690406  2.3060319260862632 10.8612336967246375   F   F   F
  2.2329631891986130  2.5482853542132564 11.6081185941916676   F   F   F
```

3.3879756472422886	1.3729304971330487	9.5654178022134726	F	F	F
-0.6099308659384719	3.6572354808710319	10.2987723773365918	F	F	F
1.0741325945506290	3.3398253655638945	8.2518078419286898	F	F	F
-0.1896947466424452	1.6706579310542629	11.9218080039603880	F	F	F
2.5359672684976289	-0.0436034517072260	14.5050718430130114	F	F	F
1.1878541204003157	1.9555643495174622	12.6701466762358965	F	F	F
-1.3312994995517764	2.1912357006718826	16.3541107227848386	T	T	T
2.0075734684757989	2.4168019004341490	16.9745037013736138	T	T	T
3.4970656085392617	1.0832608036090119	15.1743557121126642	T	T	T
1.6890504217365268	0.5845574440269169	13.2917821082657621	F	F	F
-0.8302313865181832	3.5844727253916839	15.6943498514980497	T	T	T
1.0284122964577835	2.9908036747796589	13.8903255655927058	F	F	F
-0.3999707118413574	1.6389087477093545	17.5728646269021809	T	T	T
0.0302984808711893	4.0599703903748567	19.9048726929548856	T	T	T
1.0898459351998728	1.8407812539607076	18.1877132674985020	T	T	T
4.0123259472337676	1.8558848430616564	21.8785057892607249	T	T	T
3.6257109781746042	1.0327036875784736	20.5339658170659121	T	T	T
1.6656531299213584	0.4418596040046273	18.7819949690228469	T	T	T
-1.2036654328078631	3.5002244583364450	20.7993519697712159	T	T	T
1.0424766169205701	2.8786856719785940	19.4393429918287026	T	T	T
0.3088683929550181	2.2265963864206793	22.6447669599897807	T	T	T
2.7912403427363293	1.7751806086694806	22.9938260751957770	T	T	T
1.3398502426699208	0.6617262763903743	8.0000000000000018	F	F	F
1.1444514604801637	1.6069964979926934	8.0158744918591101	F	F	F
1.9196681843552341	3.7339507153633393	8.0308754104330919	F	F	F
0.0756447124823282	4.3590604822697836	9.0169746245084834	F	F	F
-3.6256803045263264	6.4865314691886802	10.8612336967246375	F	F	F
-0.1806493473586732	6.7287848973156743	11.6081185941916676	F	F	F
0.9743631106850024	5.5534300402354653	9.5654178022134726	F	F	F
-3.0235434024957577	7.8377350239734476	10.2987723773365918	F	F	F
-1.3394799420066570	7.5203249086663115	8.2518078419286898	F	F	F
-2.6033072831997317	5.8511574741566790	11.9218080039603880	F	F	F
0.1223547319403430	4.1368960913951902	14.5050718430130114	F	F	F
-1.2257584161569703	6.1360638926198785	12.6701466762358965	F	F	F
-3.7912063155066473	6.3712885229067764	16.3569588178065075	T	T	T
-0.4943727382618510	6.7277553345397489	16.8912797183611367	T	T	T
1.0611500304378170	5.2867267494256245	15.1864475807197383	T	T	T
-0.7245621148207592	4.7650569871293333	13.2917821082657621	F	F	F
-3.2855197906975637	7.7697837371067839	15.6893441485432596	T	T	T
-1.3852002400995025	7.1713032178820759	13.8903255655927058	F	F	F
-2.8448282068749906	5.8395980039155164	17.5677308979932114	T	T	T
-2.2460441536446809	8.2650077072253794	20.0236728575287479	T	T	T
-1.3447392872575961	6.0784272401889323	18.1211986147366737	T	T	T
0.8926367865927973	6.3133987256185522	21.8572695136436330	T	T	T
0.8884271936930805	5.0752503018308994	20.8152155887892931	T	T	T
-0.6388790940846240	4.6901706675870827	18.5665553061400459	T	T	T
-3.1689695997790452	7.8466838892578306	21.2945051194605313	T	T	T
-1.3763395074401574	7.0168928784480213	19.4493217174948896	T	T	T
-2.8957299486729076	5.5829731133892819	22.8379208185901987	T	T	T
-0.4964916877370024	6.6379450107160221	22.6339016937409276	T	T	T
-1.0737622938873650	4.8422258194927910	8.0000000000000018	F	F	F
-1.2691610760771224	5.7874960410951104	8.0158744918591101	F	F	F
-0.4939443522020517	7.9144502584657550	8.0308754104330919	F	F	F
7.3164823221541884	0.1785609391673665	9.0169746245084834	F	F	F
3.6151573051455341	2.3060319260862632	10.8612336967246375	F	F	F
7.0601882623131873	2.5482853542132564	11.6081185941916676	F	F	F
8.2152007203568616	1.3729304971330487	9.5654178022134726	F	F	F
4.2172942071761028	3.6572354808710319	10.2987723773365918	F	F	F
5.9013576676652040	3.3398253655638945	8.2518078419286898	F	F	F
4.6375303264721293	1.6706579310542629	11.9218080039603880	F	F	F
7.3631923416122040	-0.0436034517072260	14.5050718430130114	F	F	F
6.0150791935148895	1.9555643495174622	12.6701466762358965	F	F	F
3.4935613537564247	2.1963024204376422	16.3602644644395383	T	T	T

6.8502025857945776	2.4905327857714017	16.9575445666083127	T	T	T
8.3258314123927732	1.0889654660231638	15.1598103882123247	T	T	T
6.5162754948511017	0.5845574440269169	13.2917821082657621	F	F	F
3.9769258758404273	3.5950769741384070	15.6923325337869972	T	T	T
5.8556373695723583	2.9908036747796589	13.8903255655927058	F	F	F
4.4501898172566294	1.7267060980849884	17.5904199874984251	T	T	T
4.7638991710029108	4.2181505595632505	20.0791021566852024	T	T	T
5.9103274507829395	2.0742414459790797	18.2154265075772983	T	T	T
8.5123702924770051	2.3330515140570296	21.9224121495068793	T	T	T
8.1334423460839087	0.9530062212365948	21.1629680028478191	T	T	T
6.5111650813600308	0.7852194605960550	18.9692980679510370	T	T	T
4.1638738154371504	3.4115994163339343	21.3707733580396777	T	T	T
5.8333635625691969	3.2805775985081405	19.2994188811056944	T	T	T
5.3194927730846162	1.2627849064651142	22.6512687151822227	T	T	T
7.4770712937942694	2.8451230072368001	23.1393281692090440	T	T	T
6.1670753157844951	0.6617262763903743	8.0000000000000018	F	F	F
5.9716765335947377	1.6069964979926934	8.0158744918591101	F	F	F
6.7468932574698091	3.7339507153633393	8.0308754104330919	F	F	F
4.9028697855969030	4.3590604822697836	9.0169746245084834	F	F	F
1.2015447685882479	6.4865314691886802	10.8612336967246375	F	F	F
4.6465757257559011	6.7287848973156743	11.6081185941916676	F	F	F
5.8015881837995771	5.5534300402354653	9.5654178022134726	F	F	F
1.8036816706188166	7.8377350239734476	10.2987723773365918	F	F	F
3.4877451311079177	7.5203249086663115	8.2518078419286898	F	F	F
2.2239177899148435	5.8511574741566790	11.9218080039603880	F	F	F
4.9495798050549178	4.1368960913951902	14.5050718430130114	F	F	F
3.6014666569576042	6.1360638926198785	12.6701466762358965	F	F	F
1.0079817826287358	6.4364537429576769	16.3390162038522355	T	T	T
4.3849824552424197	6.5318932444707212	17.0118940773735439	T	T	T
5.8971929106613015	5.2833947047507541	15.1496216208288974	T	T	T
4.1026629582938146	4.7650569871293333	13.2917821082657621	F	F	F
1.5416742848125091	7.8122753014087856	15.6762825639627721	T	T	T
3.4420248330150716	7.1713032178820759	13.8903255655927058	F	F	F
1.9026417632648218	6.0309235840157474	17.6311858622562809	T	T	T
2.4850036759200358	8.3638744371293168	20.1369127908402028	T	T	T
3.3942673810957991	6.1577329028787036	18.2546880937508256	T	T	T
5.7927042988700190	6.5063197966295583	21.9000210251086500	T	T	T
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1.3942523917281213	7.5782270885395109	21.0125908416910647	T	T	T
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2.0164191033630336	5.9403109143957122	23.0314818602923168	T	T	T
4.4942288373042141	6.9348068227286905	22.8373606819473487	T	T	T
3.7534627792272097	4.8422258194927910	8.0000000000000018	F	F	F
3.5580639970374524	5.7874960410951104	8.0158744918591101	F	F	F
4.3332807209125228	7.9144502584657550	8.0308754104330919	F	F	F
-0.0330779162189924	-0.4037748136351681	24.6056081263898889	T	T	T
2.5795214707487992	0.3310140223366065	24.6020823048684960	T	T	T
7.7371085110159283	1.5350210354878324	24.7261620807673843	T	T	T
0.6325595243035319	2.2089111316214671	24.6072783021289752	T	T	T
3.2892301861123929	2.8615786459248667	24.6600121983775509	T	T	T
-1.1642445436133739	4.1035123104018929	24.6953487645265213	T	T	T
1.4623987114403312	4.7894623643956171	24.6550844965735045	T	T	T
4.0938758704775529	5.4293885903109480	24.6290713255038476	T	T	T
-0.4404319398398672	6.7140539730869389	24.6102920396791944	T	T	T
2.1858427488109529	7.3142453749151670	24.6634359024553689	T	T	T
8.1304604135825951	0.0404257355843719	26.7656289867446908	T	T	T
1.0650752515095681	0.7103884131863174	26.7417765856849172	T	T	T
6.2534908476264155	1.9798747818517552	26.8363417652695802	T	T	T
-0.7780571041068500	2.6220147812135539	26.8386233429177459	T	T	T
1.7972683737453030	3.2789458103053031	26.7630282348470523	T	T	T
-0.0487050348128400	5.2189228375479733	26.7572897375742151	T	T	T
2.5628736466753304	5.8451967550272181	26.8584332439814197	T	T	T

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  0.6877811438010192  7.7820154465575211 26.7568760415832827   T   T   T
 -3.3779560790612777  7.5795319947539035 28.9408001066356562   T   T   T
 -0.3950964779860300  1.1286694551177887 28.9486278704173152   T   T   T
  2.2014534346827572  1.7779605402375409 28.9584972093776862   T   T   T
  7.3905025777927218  3.0625903390505274 28.9739933306937303   T   T   T
  0.3392485093884095  3.7108784825179826 28.9400761809034606   T   T   T
  2.9340738313584138  4.3430782028213022 28.9535569964602786   T   T   T
 -1.5098209603491373  5.6487174399374114 28.9541602124220532   T   T   T
  1.0756493217041991  6.2826972716181526 28.9636913808019223   T   T   T
  3.6802201645696875  6.9054329933315808 28.9888101657729642   T   T   T
  6.6527361398370362  0.4869029732774947 28.9442157753765272   T   T   T
  5.1883092988873658  0.9362218552552387 24.6177626110708303   T   T   T
  5.8955806917264209  3.4857547339090247 24.6733857771898926   T   T   T
 -2.9788776095647838  6.0457186041280622 24.7237833127775382   T   T   T
 -1.8926394963439941  7.1710767703383533 26.7517628332567234   T   T   T
  3.6701319212990269  1.3534691485561983 26.8169376653959119   T   T   T
  4.4024361524925677  3.9288733477388069 26.7369080036147473   T   T   T
 -2.6457782564373926  4.5737429221758159 26.8552059035657464   T   T   T
  5.1678412869264134  6.5026844624870481 26.8113655273832912   T   T   T
  4.0563527245223119 -0.1454718956349783 28.9495191679748416   T   T   T
  4.7915468020470238  2.4230503515203727 28.9532210462834634   T   T   T
  5.5412075046263434  5.0137378461435871 28.9654837431114807   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Rh E_tot= -883.22668798 eV
 D3-zero damping= -9.572258 eV, D3-BJ damping= -13.6065172 eV
Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H
O  H Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     9.6544501462291485    0.0000000000000000    0.0000000000000000
    -4.8272250731145716    8.3609990862048331    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.9467803099241330
   2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.4892572490396141  0.1785609391673665  9.0169746245084816   F   F   F
 -1.2120677679690406  2.3060319260862632 10.8612336967246357   F   F   F
  2.2329631891986130  2.5482853542132564 11.6081185941916623   F   F   F
  3.3879756472422886  1.3729304971330487  9.5654178022134708   F   F   F
 -0.6099308659384719  3.6572354808710319 10.2987723773365900   F   F   F
  1.0741325945506290  3.3398253655638945  8.2518078419286844   F   F   F
 -0.1896947466424452  1.6706579310542629 11.9218080039603862   F   F   F
  2.5359672684976289 -0.0436034517072260 14.5050718430130097   F   F   F
  1.1878541204003157  1.9555643495174622 12.6701466762358947   F   F   F
 -1.3639083507119529  2.2075095360750860 16.3474873641441896   T   T   T
  1.9683579291223805  2.4030502269003526 16.9400408949629160   T   T   T
  3.5056489002858040  1.0747248656572994 15.1821334226480928   T   T   T
  1.6890504217365268  0.5845574440269169 13.2917821082657603   F   F   F
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  1.0284122964577835  2.9908036747796589 13.8903255655927005   F   F   F
 -0.4491655480658381  1.7896370516342213 17.6198997993024840   T   T   T
 -0.1967504502208831  3.9305621779333384 20.0680649689371968   T   T   T
  1.0395364697437304  2.0365049567868749 18.2185292738874729   T   T   T
  3.3427468328098029  1.8983163306493367 21.9366859321046519   T   T   T
  2.6430733881714947  0.5151606820330505 21.4368102478070810   T   T   T
  1.4467852912238635  0.6877471063027005 19.0051365355865904   T   T   T
 -1.1544039698592050  2.7264995118488131 20.5775124508849032   T   T   T
  1.0676891011878376  3.2769117657653446 19.2785767299386386   T   T   T
 -0.1091670624760096  1.5012517852394589 22.7545424755841452   T   T   T
  2.3426212892530152  2.7805665189532021 22.8922242770764406   T   T   T
  1.4170687242149738  2.4187088095361284 22.9467803099241330   T   T   T
 -0.0087192259192668  0.5253386230628647 22.9000330446501863   T   T   T
  1.3398502426699208  0.6617262763903743  8.0000000000000000   F   F   F
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1.1444514604801637	1.6069964979926934	8.0158744918591047	F	F	F
1.9196681843552341	3.7339507153633393	8.0308754104330866	F	F	F
0.0756447124823283	4.3590604822697827	9.0169746245084816	F	F	F
-3.6256803045263264	6.4865314691886802	10.8612336967246357	F	F	F
-0.1806493473586728	6.7287848973156734	11.6081185941916623	F	F	F
0.9743631106850028	5.5534300402354653	9.5654178022134708	F	F	F
-3.0235434024957577	7.8377350239734485	10.2987723773365900	F	F	F
-1.3394799420066568	7.5203249086663106	8.2518078419286844	F	F	F
-2.6033072831997308	5.8511574741566790	11.9218080039603862	F	F	F
0.1223547319403431	4.1368960913951902	14.5050718430130097	F	F	F
-1.2257584161569701	6.1360638926198785	12.6701466762358947	F	F	F
-3.7775208872692385	6.3880090791775022	16.3474873641441896	T	T	T
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1.0920363637285182	5.2552244087597160	15.1821334226480928	T	T	T
-0.7245621148207591	4.7650569871293333	13.2917821082657603	F	F	F
-3.2865644432266139	7.7807225939205393	15.6752459533803243	T	T	T
-1.3852002400995023	7.1713032178820750	13.8903255655927005	F	F	F
-2.8627780846231241	5.9701365947366378	17.6198997993024840	T	T	T
-2.6103629867781688	8.1110617210357550	20.0680649689371968	T	T	T
-1.3740760668135554	6.2170044998892919	18.2185292738874729	T	T	T
0.9291342962525171	6.0788158737517533	21.9366859321046519	T	T	T
0.2294608516142089	4.6956602251354669	21.4368102478070810	T	T	T
-0.9668272453334223	4.8682466494051173	19.0051365355865904	T	T	T
-3.5680165064164910	6.9069990549512301	20.5775124508849032	T	T	T
-1.3459234353694483	7.4574113088677612	19.2785767299386386	T	T	T
-2.5227795990332953	5.6817513283418757	22.7545424755841452	T	T	T
-0.0709912473042706	6.9610660620556182	22.8922242770764406	T	T	T
-0.9965438123423120	6.5992083526385450	22.9467803099241330	T	T	T
-2.4223317624765528	4.7058381661652815	22.9000330446501863	T	T	T
-1.0737622938873650	4.8422258194927910	8.0000000000000000	F	F	F
-1.2691610760771221	5.7874960410951104	8.0158744918591047	F	F	F
-0.4939443522020517	7.9144502584657559	8.0308754104330866	F	F	F
7.3164823221541884	0.1785609391673665	9.0169746245084816	F	F	F
3.6151573051455337	2.3060319260862632	10.8612336967246357	F	F	F
7.0601882623131873	2.5482853542132564	11.6081185941916623	F	F	F
8.2152007203568633	1.3729304971330487	9.5654178022134708	F	F	F
4.2172942071761028	3.6572354808710319	10.2987723773365900	F	F	F
5.9013576676652031	3.3398253655638945	8.2518078419286844	F	F	F
4.6375303264721293	1.6706579310542629	11.9218080039603862	F	F	F
7.3631923416122032	-0.0436034517072260	14.5050718430130097	F	F	F
6.0150791935148895	1.9555643495174622	12.6701466762358947	F	F	F
3.4633167224026211	2.2075095360750860	16.3474873641441896	T	T	T
6.7955830022369543	2.4030502269003526	16.9400408949629160	T	T	T
8.3328739734003783	1.0747248656572994	15.1821334226480928	T	T	T
6.5162754948511008	0.5845574440269169	13.2917821082657603	F	F	F
3.9542731664452462	3.6002230508181228	15.6752459533803243	T	T	T
5.8556373695723583	2.9908036747796589	13.8903255655927005	F	F	F
4.3780595250487364	1.7896370516342213	17.6198997993024840	T	T	T
4.6304746228936908	3.9305621779333384	20.0680649689371968	T	T	T
5.8667615428583044	2.0365049567868749	18.2185292738874729	T	T	T
8.1699719059243776	1.8983163306493367	21.9366859321046519	T	T	T
7.4702984612860686	0.5151606820330505	21.4368102478070810	T	T	T
6.2740103643384373	0.6877471063027005	19.0051365355865904	T	T	T
3.6728211032553695	2.7264995118488131	20.5775124508849032	T	T	T
5.8949141743024116	3.2769117657653446	19.2785767299386386	T	T	T
4.7180580106385648	1.5012517852394589	22.7545424755841452	T	T	T
7.1698463623675899	2.7805665189532021	22.8922242770764406	T	T	T
6.2442937973295480	2.4187088095361284	22.9467803099241330	T	T	T
4.8185058471953077	0.5253386230628647	22.9000330446501863	T	T	T
6.1670753157844951	0.6617262763903743	8.0000000000000000	F	F	F
5.9716765335947377	1.6069964979926934	8.0158744918591047	F	F	F
6.7468932574698082	3.7339507153633393	8.0308754104330866	F	F	F
4.9028697855969021	4.3590604822697827	9.0169746245084816	F	F	F

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  1.2015447685882479  6.4865314691886802 10.8612336967246357   F   F   F
  4.6465757257559019  6.7287848973156734 11.6081185941916623   F   F   F
  5.8015881837995771  5.5534300402354653  9.5654178022134708   F   F   F
  1.8036816706188166  7.8377350239734485 10.2987723773365900   F   F   F
  3.4877451311079177  7.5203249086663106  8.2518078419286844   F   F   F
  2.2239177899148435  5.8511574741566790 11.9218080039603862   F   F   F
  4.9495798050549169  4.1368960913951902 14.5050718430130097   F   F   F
  3.6014666569576042  6.1360638926198785 12.6701466762358947   F   F   F
  1.0497041858453355  6.3880090791775022 16.3474873641441896   T   T   T
  4.3819704656796690  6.5835497700027688 16.9400408949629160   T   T   T
  5.9192614368430920  5.2552244087597160 15.1821334226480928   T   T   T
  4.1026629582938154  4.7650569871293333 13.2917821082657603   F   F   F
  1.5406606298879604  7.7807225939205393 15.6752459533803243   T   T   T
  3.4420248330150720  7.1713032178820750 13.8903255655927005   F   F   F
  1.9644469884914504  5.9701365947366378 17.6198997993024840   T   T   T
  2.2168620863364055  8.1110617210357550 20.0680649689371968   T   T   T
  3.4531490063010191  6.2170044998892919 18.2185292738874729   T   T   T
  5.7563593693670914  6.0788158737517533 21.9366859321046519   T   T   T
  5.0566859247287832  4.6956602251354669 21.4368102478070810   T   T   T
  3.8603978277811519  4.8682466494051173 19.0051365355865904   T   T   T
  1.2592085666980835  6.9069990549512301 20.5775124508849032   T   T   T
  3.4813016377451262  7.4574113088677612 19.2785767299386386   T   T   T
  2.3044454740812790  5.6817513283418757 22.7545424755841452   T   T   T
  4.7562338258103036  6.9610660620556182 22.8922242770764406   T   T   T
  3.8306812607722622  6.5992083526385450 22.9467803099241330   T   T   T
  2.4048933106380215  4.7058381661652815 22.9000330446501863   T   T   T
  3.7534627792272093  4.8422258194927910  8.0000000000000000   F   F   F
  3.5580639970374524  5.7874960410951104  8.0158744918591047   F   F   F
  4.3332807209125228  7.9144502584657559  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Rh E_tot= -277.28069999 eV
 D3-zero damping= -14.0778022 eV, D3-BJ damping= -16.9893653 eV
Rh
 1.0000000000000000
     9.6544501462291485    0.0000000000000000    0.0000000000000000
    -4.8272250731145716    8.3609990862048331    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000595648638128 -0.0000085203602106  8.1230690787395101
  2.5998163836544905  0.6455386810131792  8.1287576323857706
  7.7955095430323054  1.9286988041673827  8.1287392128467655
  0.7405145685190203  2.5735756149399247  8.1285748837571195
  3.3415484227378824  3.2155913323643102  8.1291824235854939
 -1.1140254899281161  4.5019013223224000  8.1280897812842809
  1.4855724006486479  5.1451698620332182  8.1281399197442923
  4.0864906795501863  5.7868029449552409  8.1288083134268696
 -0.3713634255742174  7.0747957555630103  8.1281180786926193
  2.2282499240553886  7.7154348156918413  8.1284876832066804
  8.1709119259437291  0.4294531318497110 10.2735233912507216
  1.1138757216666775  1.0701008504778671 10.2735315212716234
  6.3108709375801837  2.3575100658463830 10.2757993369002971
 -0.7447230087870993  3.0025300096002385 10.2746158781096337
  1.8546910249098179  3.6433991225840110 10.2747762659344328
  0.0000045729888670  5.5739818226771725 10.2740833696928888
  2.5994441761340434  6.2149583195965041 10.2747510914237896
  0.7445772328021770  8.1455342145698033 10.2746051699363825
 -3.3414595495415580  7.9325917347971941 12.4203356308503086
 -0.3717990720693223  1.5008020276200185 12.4203067105500331
  2.2274251586084919  2.1415938537880486 12.4206670701707047
  7.4263656801983613  3.4324114326535562 12.4206793596118708
  0.3715232362571894  4.0735301490339522 12.4209961814629661
  2.9688913989359289  4.7150478358545316 12.4207024776054986
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 -1.4853569867798770  6.0026513886511967 12.4208756731908121
  1.1137498373307297  6.6461036709587606 12.4209630410783003
  3.7134475550966561  7.2886206563388818 12.4202532221798183
  6.6861700889445252  0.8580621426428959 12.4206294822331493
  5.1989187027395287  1.2859190519408177  8.1291817630956889
  5.9412556514895405  3.8593803239334554  8.1291634922416840
 -2.9686756174601605  6.4329216120338453  8.1286117568021901
 -1.8545850998154769  7.5047023123500827 10.2746273944173563
  3.7135541740037299  1.7169328786401377 10.2758447556461530
  4.4574249902453067  4.2865053699543330 10.2758309839117992
 -2.5992009342452773  4.9330403250247992 10.2746067046675886
  5.1969182372625147  6.8613896043097515 10.2735048923818457
  4.0866531965823611  0.2134413703448029 12.4207834110590145
  4.8273764954661296  2.7869455810838399 12.4262439433424454
  5.5683431582806442  5.3611697492689316 12.4206755223701730

Interface: O-a-SiO2(0001)/fcc(111)_sqrt13/Os E_tot= -1275.84675406 eV
 D3-zero damping= -25.9692514 eV, D3-BJ damping= -32.7051063 eV
Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O
Si  O  H Os
 1.0000000000000000
     9.7653265728439838    0.0000000000000000    0.0000000000000000
    -4.8826632864219892    8.4570208883341191    0.0000000000000000
     0.0000000000000023    0.0000000000000039   37.0209043940043188
   2   5   3   6   3   7   2   2   5   3   6   3   7   2   2   5   3   6
3   7   2   2   5   3   6   3   7   2  39
Selective dynamics
Cartesian
  2.5178450965625920  0.1806116203110874  9.0169746245084816   F   F   F
 -1.2259877469312725  2.3325155244011841 10.8612336967246357   F   F   F
  2.2586076304076763  2.5775511093614596 11.6081185941916658   F   F   F
  3.4268848163337080  1.3886979023406973  9.5654178022134708   F   F   F
 -0.6169356102660154  3.6992369615629528 10.2987723773365900   F   F   F
  1.0864684585294608  3.3781815532744850  8.2518078419286880   F   F   F
 -0.1918732938757680  1.6898445837051521 11.9218080039603862   F   F   F
  2.5650915567257910 -0.0441042150692139 14.5050718430130097   F   F   F
  1.2014960179931202  1.9780230068004501 12.6701466762358947   F   F   F
 -1.3217606934957147  2.1849089744878354 16.3197841070459049   T   T   T
  2.0390979080645102  2.4358129331307672 16.9680677619170162   T   T   T
  3.5233199848382180  1.0685469067104989 15.2060488438219963   T   T   T
  1.7084483027445481  0.5912707875693368 13.2917821082657603   F   F   F
 -0.8317386123761179  3.5982745288244073 15.6834650955149417   T   T   T
  1.0402230861755730  3.0251515267177207 13.8903255655927040   F   F   F
 -0.3864569379885457  1.6771265758771046 17.5536953218004612   T   T   T
  0.0513795292937967  4.2135068842071295 19.9093619592073594   T   T   T
  1.0905389436643242  1.9219941517240224 18.1848301529887060   T   T   T
  4.0885695881142219  2.1309351652460240 21.7963379290425046   T   T   T
  3.6361397994031734  1.3054482456652967 20.4667624234406951   T   T   T
  1.6306523204279628  0.5491860556135623 18.8693636650208774   T   T   T
 -1.0196094254481491  3.6399607515482839 20.9883883751817208   T   T   T
  1.0215194275146435  3.0399736552365781 19.3608751966341366   T   T   T
  0.3023984016329201  1.9991412642437854 22.7017779355179172   T   T   T
  2.8491486513471651  2.5552794173896292 22.7570259915186561   T   T   T
  1.3552377380586960  0.6693258645400899  8.0000000000000000   F   F   F
  1.1575949007020525  1.6254520316151413  8.0158744918591083   F   F   F
  1.9417145925238684  3.7768332313227888  8.0308754104330902   F   F   F
  0.0765134533515969  4.4091220644781473  9.0169746245084816   F   F   F
 -3.6673193901422669  6.5610259685682442 10.8612336967246357   F   F   F
 -0.1827240128033185  6.8060615535285196 11.6081185941916658   F   F   F
  0.9855531731227130  5.6172083465077565  9.5654178022134708   F   F   F
 -3.0582672534770103  7.9277474057300115 10.2987723773365900   F   F   F
 -1.3548631846815340  7.6066919974415441  8.2518078419286880   F   F   F
 -2.6332049370867634  5.9183550278722112 11.9218080039603862   F   F   F
```

0.1237599135147965	4.1844062290978457	14.5050718430130097	F	F	F
-1.2398356252178746	6.2065334509675099	12.6701466762358947	F	F	F
-3.8466917089036055	6.4671733904005686	16.3547357449459270	T	T	T
-0.4617993703356846	6.7773899228772070	16.8678080748870087	T	T	T
1.0640093383666656	5.3400917413216176	15.1605159978103856	T	T	T
-0.7328833404664467	4.8197812317363971	13.2917821082657603	F	F	F
-3.3463661186856783	7.8456472940767199	15.6471975697453036	T	T	T
-1.4011085570354218	7.2536619708847807	13.8903255655927040	F	F	F
-2.8643174060823084	6.0475725677188157	17.5800458554151433	T	T	T
-2.1922864280287406	8.5224188260889981	20.0158608635612474	T	T	T
-1.3573631602139398	6.2615395810093695	18.1262723096106697	T	T	T
0.9656185126738032	6.3804345473895667	21.8602953264255433	T	T	T
0.9886576377249957	5.2968929553669701	20.6581272790649422	T	T	T
-0.7779876238546297	4.8478539661095992	18.6702173861897904	T	T	T
-2.9431560646039840	7.9940150113250050	21.3628077690502387	T	T	T
-1.2971863539182351	7.3329491642705413	19.3540068372677219	T	T	T
-3.1464136235567990	5.6500104520892309	22.7777559441539452	T	T	T
-0.4592945703560695	6.5293657854632041	22.6349009473642795	T	T	T
-1.0860939051522986	4.8978363087071495	8.0000000000000000	F	F	F
-1.2837367425089423	5.8539624757822004	8.0158744918591083	F	F	F
-0.4996170506871264	8.0053436754898470	8.0308754104330902	F	F	F
7.4005083829845839	0.1806116203110874	9.0169746245084816	F	F	F
3.6566755394907200	2.3325155244011841	10.8612336967246357	F	F	F
7.1412709168296686	2.5775511093614596	11.6081185941916658	F	F	F
8.3095481027556986	1.3886979023406973	9.5654178022134708	F	F	F
4.2657276761559775	3.6992369615629528	10.2987723773365900	F	F	F
5.9691317449514534	3.3781815532744850	8.2518078419286880	F	F	F
4.6907899925462244	1.6898445837051521	11.9218080039603862	F	F	F
7.4477548431477842	-0.0441042150692139	14.5050718430130097	F	F	F
6.0841593044151123	1.9780230068004501	12.6701466762358947	F	F	F
3.5261677593673837	2.2295471595507315	16.3499858007246388	T	T	T
6.9474492180397149	2.3840540986817635	16.8943685118695726	T	T	T
8.4460035105527176	1.0745269623145537	15.1342548575133193	T	T	T
6.5911115891665402	0.5912707875693368	13.2917821082657603	F	F	F
3.9979802112081586	3.6146943474924225	15.6494017952679805	T	T	T
5.9228863725975653	3.0251515267177207	13.8903255655927040	F	F	F
4.5042895602239357	1.8311254160963570	17.5871490992320254	T	T	T
5.0406607311163825	4.4310100407399649	19.9493235789489454	T	T	T
5.9870397285651658	2.1457578964866917	18.1776908717322740	T	T	T
8.6870323733170789	2.2981879619704455	21.8923042806165888	T	T	T
8.3069272495281616	1.0650424803534866	20.9305008459896769	T	T	T
6.4197320017427906	0.8666836783649927	19.0728420514421124	T	T	T
4.6931175884646903	3.5562402414432128	21.2754526517897844	T	T	T
6.0523975649228374	3.5115981581141358	19.0657112970631992	T	T	T
5.1124147855323310	1.2032671754989330	22.6868094572795691	T	T	T
7.5407817508286117	2.6254818695925306	23.0675428311348085	T	T	T
6.2379010244806876	0.6693258645400899	8.0000000000000000	F	F	F
6.0402581871240448	1.6254520316151413	8.0158744918591083	F	F	F
6.8243778789458611	3.7768332313227888	8.0308754104330902	F	F	F
4.9591767397735893	4.4091220644781473	9.0169746245084816	F	F	F
1.2153438962797249	6.5610259685682442	10.8612336967246357	F	F	F
4.6999392736186731	6.8060615535285196	11.6081185941916658	F	F	F
5.8682164595447057	5.6172083465077565	9.5654178022134708	F	F	F
1.8243960329449820	7.9277474057300115	10.2987723773365900	F	F	F
3.5278001017404583	7.6066919974415441	8.2518078419286880	F	F	F
2.2494583493352294	5.9183550278722112	11.9218080039603862	F	F	F
5.0064231999367887	4.1844062290978457	14.5050718430130097	F	F	F
3.6428276612041177	6.2065334509675099	12.6701466762358947	F	F	F
1.0363760707403891	6.4869300465768491	16.3128297159565570	T	T	T
4.4373442710784436	6.6321533070889434	17.0077591965970214	T	T	T
5.9446242800020146	5.3127573756969593	15.2037773987793283	T	T	T
4.1497799459555447	4.8197812317363971	13.2917821082657603	F	F	F
1.5857673571286619	7.8727440472148515	15.6764803153663710	T	T	T

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  3.4815547293865703  7.2536619708847807 13.8903255655927040   F   F   F
  1.9443487816118457  6.0161137913877258 17.5737272050679891   T   T   T
  2.4609210931645999  8.5026980845131455 20.1250135456538750   T   T   T
  3.4158585890802340  6.2365457461029878 18.2214820957270227   T   T   T
  5.8790913820134172  6.7348652284743862 21.8041957455191877   T   T   T
  5.6226946937131936  5.8717537666938364 20.4386365682200193   T   T   T
  3.7909605730278511  4.8316224583433662 18.9689149470402008   T   T   T
  1.5286156771861896  7.7483375743324787 21.2141539445290341   T   T   T
  3.3841218741676418  7.4525564600238159 19.3029632459257634   T   T   T
  2.0389561134139913  5.8296328847193815 23.0415279404155946   T   T   T
  4.6003438058641262  7.3582231856249871 22.6333225810950722   T   T   T
  3.7965693812696935  4.8978363087071495  8.0000000000000000   F   F   F
  3.5989265439130502  5.8539624757822004  8.0158744918591083   F   F   F
  4.3830462357348656  8.0053436754898470  8.0308754104330902   F   F   F
 -0.2149133675262020 -0.6959896060713380 24.6245198055786609   T   T   T
  2.3997105682914959 -0.0031798603298196 24.7351237211157411   T   T   T
  7.6336413949971789  1.2971181806008198 24.7459276246894753   T   T   T
  0.5003974716502674  1.9513844217274150 24.6745132597820955   T   T   T
  3.0993316170163250  2.6101335868703481 24.7061320292086002   T   T   T
 -1.3783056316759268  3.8662452373531964 24.7503275591967622   T   T   T
  1.2893392692365846  4.5926829722086806 24.7256921354934036   T   T   T
  3.8878194116435014  5.2021725683595754 24.7618786245996070   T   T   T
 -0.6044045676287702  6.5268439518182548 24.6506207204409513   T   T   T
  2.0289524401185677  7.1610138664421941 24.7259381123872402   T   T   T
  8.0570720203432966 -0.2345262390742192 26.8539968744571986   T   T   T
  0.8841138956401454  0.4194979379059882 26.8338794617133622   T   T   T
  6.1253247478279764  1.7140725602449738 26.8435489923663013   T   T   T
 -0.9688845030497111  2.3810462949369704 26.8336984122788493   T   T   T
  1.6241121984530282  3.0436309247573186 26.8405511376239829   T   T   T
 -0.2278041998881571  4.9793423445124700 26.8246811251737007   T   T   T
  2.3858155088353024  5.6396436953043994 26.8683686812899651   T   T   T
  0.4978057903766409  7.5918237575268517 26.8131395444966145   T   T   T
 -3.6010524926078054  7.3697448128144618 29.0080432265788311   T   T   T
 -0.6030656332743868  0.8646652404441216 29.0100462043800711   T   T   T
  2.0211589245410431  1.5160033770814325 28.9960003601665548   T   T   T
  7.2789917717275143  2.8119288268972458 29.0211779559961727   T   T   T
  0.1349630519499482  3.4743131286717910 29.0079933105148982   T   T   T
  2.7670318121218558  4.1231473794906082 29.0114682522892089   T   T   T
 -1.7473758150386307  5.4242215645071825 29.0085570467783498   T   T   T
  0.8979182342264921  6.0698625830337454 29.0127931912681341   T   T   T
  3.5145832473399778  6.7123348121833537 29.0174797396727904   T   T   T
  6.5362604809371145  0.2152735688319801 28.9962296258546779   T   T   T
  5.0218913994860026  0.6966431194277077 24.6204722939073086   T   T   T
  5.7807447154202976  3.2622691227943608 24.7736086176507051   T   T   T
 -3.2045946989987870  5.8314726020872856 24.7148733392268873   T   T   T
 -2.1201561937712201  6.9584591983928892 26.8404784647825778   T   T   T
  3.5439571521074886  1.0737170846769368 26.8195684054514452   T   T   T
  4.2869421839269792  3.6885198088334814 26.8334114055747968   T   T   T
 -2.8635114847535061  4.3257349864996089 26.8669569559811201   T   T   T
  5.0359801467219389  6.3044613131296563 26.8192410112507034   T   T   T
  3.9070788546226130 -0.4312185734613461 28.9981517630794094   T   T   T
  4.6496511111161203  2.1569315907374045 29.0128553888403147   T   T   T
  5.3968386628450160  4.7633029727059384 29.0194942478504991   T   T   T

Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Os E_tot= -884.30606268 eV
 D3-zero damping= -9.3476318 eV, D3-BJ damping= -13.2851963 eV
Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H
O  H Si  O Si  O Si  O  H  O  H
 1.0000000000000000
     9.7653265728439838    0.0000000000000000    0.0000000000000000
    -4.8826632864219892    8.4570208883341191    0.0000000000000000
     0.0000000000000019    0.0000000000000033   30.9052895435168544
```

```
   2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
2   5   3   6   3   6   2   1   2   2   5   3   6   3   6   2   1   2
Selective dynamics
Cartesian
  2.5178450965625920  0.1806116203110874  9.0169746245084816   F   F   F
 -1.2259877469312725  2.3325155244011841 10.8612336967246357   F   F   F
  2.2586076304076763  2.5775511093614596 11.6081185941916623   F   F   F
  3.4268848163337080  1.3886979023406973  9.5654178022134708   F   F   F
 -0.6169356102660154  3.6992369615629528 10.2987723773365900   F   F   F
  1.0864684585294608  3.3781815532744850  8.2518078419286844   F   F   F
 -0.1918732938757680  1.6898445837051521 11.9218080039603862   F   F   F
  2.5650915567257910 -0.0441042150692139 14.5050718430130097   F   F   F
  1.2014960179931202  1.9780230068004501 12.6701466762358947   F   F   F
 -1.3687986342767942  2.2257793513003756 16.3367251418463830   T   T   T
  2.0258227826926434  2.4303615543562169 16.9464077202566834   T   T   T
  3.5269422011598137  1.0777481634403401 15.1840466964595020   T   T   T
  1.7084483027445481  0.5912707875693368 13.2917821082657603   F   F   F
 -0.8760774752985868  3.6180047810518801 15.6596525543747642   T   T   T
  1.0402230861755730  3.0251515267177207 13.8903255655927005   F   F   F
 -0.4201894111455257  1.7984300302407021 17.5821746816916082   T   T   T
 -0.1959035002279492  3.9828629475565336 20.0361695886507611   T   T   T
  1.0619216032505898  2.0522079916527471 18.1962694524842377   T   T   T
  3.3757521896350511  1.9341480964068469 21.8986136488514767   T   T   T
  2.7029890041161830  0.5459010609346024 21.3779119338666170   T   T   T
  1.4817960502661116  0.6981394619803769 18.9708587031471545   T   T   T
 -1.1752642030262279  2.8066015963555251 20.5678933975941192   T   T   T
  1.0565885842613445  3.2922520773922428 19.2573265160418536   T   T   T
 -0.1230511633765138  1.5404317792915985 22.7101406697858188   T   T   T
  2.3598857133120763  2.7852408011822809 22.8633822769739119   T   T   T
  1.4335256800395255  2.4270232816245625 22.9052895435168544   T   T   T
 -0.0298859469803291  0.5705081337294245 22.8777271939335698   T   T   T
  1.3552377380586960  0.6693258645400899  8.0000000000000000   F   F   F
  1.1575949007020525  1.6254520316151413  8.0158744918591047   F   F   F
  1.9417145925238684  3.7768332313227888  8.0308754104330866   F   F   F
  0.0765134533515974  4.4091220644781473  9.0169746245084816   F   F   F
 -3.6673193901422669  6.5610259685682433 10.8612336967246357   F   F   F
 -0.1827240128033183  6.8060615535285187 11.6081185941916623   F   F   F
  0.9855531731227134  5.6172083465077574  9.5654178022134708   F   F   F
 -3.0582672534770099  7.9277474057300124 10.2987723773365900   F   F   F
 -1.3548631846815338  7.6066919974415441  8.2518078419286844   F   F   F
 -2.6332049370867625  5.9183550278722112 11.9218080039603862   F   F   F
  0.1237599135147964  4.1844062290978457 14.5050718430130097   F   F   F
 -1.2398356252178744  6.2065334509675099 12.6701466762358947   F   F   F
 -3.8101302774877888  6.4542897954674352 16.3367251418463830   T   T   T
 -0.4155088605183512  6.6588719985232760 16.9464077202566834   T   T   T
  1.0856105579488191  5.3062586076073996 15.1840466964595020   T   T   T
 -0.7328833404664465  4.8197812317363962 13.2917821082657603   F   F   F
 -3.3174091185095813  7.8465152252189396 15.6596525543747642   T   T   T
 -1.4011085570354216  7.2536619708847798 13.8903255655927005   F   F   F
 -2.8615210543565204  6.0269404744077617 17.5821746816916082   T   T   T
 -2.6372351434389438  8.2113733917235940 20.0361695886507611   T   T   T
 -1.3794100399604048  6.2807184358198072 18.1962694524842377   T   T   T
  0.9344205464240565  6.1626585405739061 21.8986136488514767   T   T   T
  0.2616573609051884  4.7744115051016625 21.3779119338666170   T   T   T
 -0.9595355929448830  4.9266499061474365 18.9708587031471545   T   T   T
 -3.6165958462372227  7.0351120405225842 20.5678933975941192   T   T   T
 -1.3847430589496501  7.5207625215593019 19.2573265160418536   T   T   T
 -2.5643828065875085  5.7689422234586578 22.7101406697858188   T   T   T
 -0.0814459298989183  7.0137512453493400 22.8633822769739119   T   T   T
 -1.0078059631714691  6.6555337257916225 22.9052895435168544   T   T   T
 -2.4712175901913236  4.7990185778964838 22.8777271939335698   T   T   T
 -1.0860939051522986  4.8978363087071495  8.0000000000000000   F   F   F
 -1.2837367425089421  5.8539624757822004  8.0158744918591047   F   F   F
```

-0.4996170506871263	8.0053436754898488	8.0308754104330866	F	F	F
7.4005083829845839	0.1806116203110874	9.0169746245084816	F	F	F
3.6566755394907196	2.3325155244011841	10.8612336967246357	F	F	F
7.1412709168296686	2.5775511093614596	11.6081185941916623	F	F	F
8.3095481027557003	1.3886979023406973	9.5654178022134708	F	F	F
4.2657276761559766	3.6992369615629528	10.2987723773365900	F	F	F
5.9691317449514525	3.3781815532744850	8.2518078419286844	F	F	F
4.6907899925462235	1.6898445837051521	11.9218080039603862	F	F	F
7.4477548431477825	-0.0441042150692139	14.5050718430130097	F	F	F
6.0841593044151123	1.9780230068004501	12.6701466762358947	F	F	F
3.5138646521451977	2.2257793513003756	16.3367251418463830	T	T	T
6.9084860691146357	2.4303615543562169	16.9464077202566834	T	T	T
8.4096054875818051	1.0777481634403401	15.1840466964595020	T	T	T
6.5911115891665402	0.5912707875693368	13.2917821082657603	F	F	F
4.0065858111234052	3.6180047810518801	15.6596525543747642	T	T	T
5.9228863725975653	3.0251515267177207	13.8903255655927005	F	F	F
4.4624738752764666	1.7984300302407021	17.5821746816916082	T	T	T
4.6867597861940427	3.9828629475565336	20.0361695886507611	T	T	T
5.9445848896725817	2.0522079916527471	18.1962694524842377	T	T	T
8.2584154760570421	1.9341480964068469	21.8986136488514767	T	T	T
7.5856522905381745	0.5459010609346024	21.3779119338666170	T	T	T
6.3644593366881033	0.6981394619803769	18.9708587031471545	T	T	T
3.7073990833957637	2.8066015963555251	20.5678933975941192	T	T	T
5.9392518706833366	3.2922520773922428	19.2573265160418536	T	T	T
4.7596121230454784	1.5404317792915985	22.7101406697858188	T	T	T
7.2425489997340682	2.7852408011822809	22.8633822769739119	T	T	T
6.3161889664615174	2.4270232816245625	22.9052895435168544	T	T	T
4.8527773394416629	0.5705081337294245	22.8777271939335698	T	T	T
6.2379010244806876	0.6693258645400899	8.0000000000000000	F	F	F
6.0402581871240439	1.6254520316151413	8.0158744918591047	F	F	F
6.8243778789458602	3.7768332313227888	8.0308754104330866	F	F	F
4.9591767397735893	4.4091220644781473	9.0169746245084816	F	F	F
1.2153438962797247	6.5610259685682433	10.8612336967246357	F	F	F
4.6999392736186731	6.8060615535285187	11.6081185941916623	F	F	F
5.8682164595447048	5.6172083465077574	9.5654178022134708	F	F	F
1.8243960329449820	7.9277474057300124	10.2987723773365900	F	F	F
3.5278001017404579	7.6066919974415441	8.2518078419286844	F	F	F
2.2494583493352294	5.9183550278722112	11.9218080039603862	F	F	F
5.0064231999367887	4.1844062290978457	14.5050718430130097	F	F	F
3.6428276612041177	6.2065334509675099	12.6701466762358947	F	F	F
1.0725330089342031	6.4542897954674352	16.3367251418463830	T	T	T
4.4671544259036402	6.6588719985232760	16.9464077202566834	T	T	T
5.9682738443708114	5.3062586076073996	15.1840466964595020	T	T	T
4.1497799459555456	4.8197812317363962	13.2917821082657603	F	F	F
1.5652541679124106	7.8465152252189396	15.6596525543747642	T	T	T
3.4815547293865703	7.2536619708847798	13.8903255655927005	F	F	F
2.0211422320654715	6.0269404744077617	17.5821746816916082	T	T	T
2.2454281429830480	8.2113733917235940	20.0361695886507611	T	T	T
3.5032532464615871	6.2807184358198072	18.1962694524842377	T	T	T
5.8170838328460484	6.1626585405739061	21.8986136488514767	T	T	T
5.1443206473271808	4.7744115051016625	21.3779119338666170	T	T	T
3.9231276934771087	4.9266499061474365	18.9708587031471545	T	T	T
1.2660674401847694	7.0351120405225842	20.5678933975941192	T	T	T
3.4979202274723420	7.5207625215593019	19.2573265160418536	T	T	T
2.3182804798344834	5.7689422234586578	22.7101406697858188	T	T	T
4.8012173565230736	7.0137512453493400	22.8633822769739119	T	T	T
3.8748573232505228	6.6555337257916225	22.9052895435168544	T	T	T
2.4114456962306683	4.7990185778964838	22.8777271939335698	T	T	T
3.7965693812696930	4.8978363087071495	8.0000000000000000	F	F	F
3.5989265439130498	5.8539624757822004	8.0158744918591047	F	F	F
4.3830462357348656	8.0053436754898488	8.0308754104330866	F	F	F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Os E_tot= -420.81793684 eV

```
 D3-zero damping= -13.927276 eV, D3-BJ damping= -16.4082713 eV
Os
 1.0000000000000000
     9.7653265728439838    0.0000000000000000    0.0000000000000000
    -4.8826632864219892    8.4570208883341191    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000580564602431  0.0000147117525127  8.1288116317869203
  2.6291109972467988  0.6511467105944518  8.1279691743055302
  7.8869236020559050  1.9512838947946729  8.1280204094859467
  0.7509139434441066  2.6024895021468915  8.1281048803221569
  3.3799875435301261  3.2526774765617423  8.1272474493063882
 -1.1268826598130040  4.5531386767420727  8.1280258250481499
  1.5030123721035495  5.2045912150296232  8.1280365222545008
  4.1320724800509128  5.8546273451230872  8.1280062246426397
 -0.3760369461908245  7.1563849670378694  8.1279941307844474
  2.2534594880658774  7.8060998178673904  8.1280987694864990
  8.2628800578295412  0.4335885595407760 10.2755173941801772
  1.1267965444002168  1.0843993930996607 10.2754102028646166
  6.3851967430090912  2.3856641413108646 10.2740080460216152
 -0.7509290784148651  3.0356859252750512 10.2746970547003862
  1.8783219543904282  3.6862081102077289 10.2746090567766473
  0.0000461613893696  5.6379993649153830 10.2742491945469006
  2.6292046739487289  6.2888193781543649 10.2746920449253416
  0.7512162092344642  8.2405421547974171 10.2745583194364798
 -3.3802556265444594  8.0226081824489039 12.4219504862423591
 -0.3749005283809244  1.5182776440462826 12.4219571036873990
  2.2544020402196647  2.1678717429065757 12.4213831492936162
  7.5122338632377481  3.4699137195857346 12.4211570652394201
  0.3760852873754901  4.1196902338042767 12.4210966177821263
  3.0042397668201155  4.7707707653702256 12.4211599393648768
 -1.5028543092660809  6.0714887253039578 12.4210903719783765
  1.1269339703543975  6.7227938652427319 12.4210846841952041
  3.7553607609439261  7.3731473021511515 12.4219801241280337
  6.7608117628949191  0.8683317992179636 12.4214131472757057
  5.2584802307299956  1.3008239358246030  8.1272402973884219
  6.0095742489885637  3.9035180926969577  8.1272503584515459
 -3.0042658433341596  6.5054814002766221  8.1280794074242966
 -1.8781496050171897  7.5895095346276236 10.2746643660085901
  3.7561838873394455  1.7344444220281932 10.2739893248828214
  4.5067035722909621  4.3368329349098849 10.2740044104415436
 -2.6294170905261662  4.9872468047325276 10.2746023829010635
  5.2584589601385296  6.9389940248238533 10.2754355124971397
  4.1316590227394903  0.2162771084611642 12.4211078007147080
  4.8827224691832365  2.8189699949915767 12.4210285413543406
  5.6329521806657539  5.4207891977545835 12.4214050407794989

Interface: O-a-SiO2(0001)/fcc(111)_sqrt13/Ru E_tot= -1200.8270642 eV
 D3-zero damping= -25.9081076 eV, D3-BJ damping= -33.0068888 eV
Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O Si  O  H Si  O Si  O
Si  O  H Ru
 1.0000000000000000
     9.6131018524371505    0.0000000000000000    0.0000000000000000
    -4.8065509262185726    8.3251904133778201    0.0000000000000000
     0.0000000000000023    0.0000000000000039   36.9476051505346703
   2   5   3   6   3   7   2   2   5   3   6   3   7   2   2   5   3   6
3   7   2   2   5   3   6   3   7   2  39
Selective dynamics
Cartesian
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  2.2233998047929497  2.5373715010268052 11.6081185941916676   F   F   F
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Oxide reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Ru E_tot= -882.68773614 eV
 D3-zero damping= -9.6522698 eV, D3-BJ damping= -13.7227116 eV
Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H  O  H Si  O Si  O Si  O  H
O  H Si  O Si  O Si  O  H  O  H
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Selective dynamics
Cartesian
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3.5996742290414190	2.2961556012692790	10.8612336967246357	F	F	F
7.0299507310115246	2.5373715010268052	11.6081185941916623	F	F	F
8.1800164760135203	1.3670504798672676	9.5654178022134708	F	F	F
4.1992322857570228	3.6415721914201415	10.2987723773365900	F	F	F
5.8760832018055824	3.3255214872137393	8.2518078419286844	F	F	F
4.6176686084556797	1.6635028001133108	11.9218080039603862	F	F	F
7.3316570977011981	-0.0434167058745553	14.5050718430130097	F	F	F
5.9893176785753024	1.9471890150314699	12.6701466762358947	F	F	F
3.4369194777722818	2.2021392984709123	16.3525138976520559	T	T	T
6.7448269820399478	2.3918710118360349	16.9388528481009111	T	T	T
8.3000370828124908	1.0749693796562592	15.1827552954867073	T	T	T
6.4883674452460252	0.5820538884056404	13.2917821082657603	F	F	F
3.9316414017622563	3.5933958321607591	15.6804969039369038	T	T	T
5.8305587156221845	2.9779945942887025	13.8903255655927005	F	F	F
4.3375305836699019	1.7817334684641997	17.6346686237423924	T	T	T
4.6007198596221786	3.9029309170749027	20.0818052193917680	T	T	T
5.8298717209797992	2.0209813307370430	18.2272506628373527	T	T	T
8.1251591876904872	1.8804094032698995	21.9569019974383970	T	T	T
7.4176216072946080	0.5011501669584718	21.4573820783851694	T	T	T
6.2373134869043163	0.6693740078468690	19.0084831543319233	T	T	T
3.6465556668119365	2.6962454132449474	20.5901407963441727	T	T	T
5.8696909787104667	3.2537426126126427	19.2962790021476565	T	T	T
4.6910774598297902	1.4829835194128793	22.7776737570096337	T	T	T
7.1296122356311056	2.7670928895591351	22.9129238998567288	T	T	T
6.2047142916644651	2.4021967362773884	22.9703660359491693	T	T	T
4.7914770378088374	0.5060015707401933	22.9218298388525774	T	T	T
6.1406628284722027	0.6588922203776907	8.0000000000000000	F	F	F
5.9461009045322895	1.6001140176530266	8.0158744918591047	F	F	F
6.7179975129822704	3.7179588682000921	8.0308754104330866	F	F	F
4.8818716658440184	4.3403914010949860	9.0169746245084816	F	F	F

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  1.1963987659321329  6.4587508079581895 10.8612336967246357   F   F   F
  4.6266752679022387  6.6999667077157152 11.6081185941916623   F   F   F
  5.7767410129042336  5.5296456865561776  9.5654178022134708   F   F   F
  1.7959568226477369  7.8041673981090511 10.2987723773365900   F   F   F
  3.4728077386962957  7.4881166939026489  8.2518078419286844   F   F   F
  2.2143931453463934  5.8260980068022210 11.9218080039603862   F   F   F
  4.9283816345919123  4.1191785008143551 14.5050718430130097   F   F   F
  3.5860422154660156  6.1097842217203802 12.6701466762358947   F   F   F
  1.0336440146629953  6.3647345051598219 16.3525138976520559   T   T   T
  4.3415515189306619  6.5544662185249454 16.9388528481009111   T   T   T
  5.8967616197032058  5.2375645863451687 15.1827552954867073   T   T   T
  4.0850919821367384  4.7446490950945508 13.2917821082657603   F   F   F
  1.5283659386529698  7.7559910388496691 15.6804969039369038   T   T   T
  3.4272832525128982  7.1405898009776125 13.8903255655927005   F   F   F
  1.9342551205606155  5.9443286751531099 17.6346686237423924   T   T   T
  2.1974443965128918  8.0655261237638136 20.0818052193917680   T   T   T
  3.4265962578705129  6.1835765374259530 18.2272506628373527   T   T   T
  5.7218837245812013  6.0430046099588095 21.9569019974383970   T   T   T
  5.0143461441853221  4.6637453736473820 21.4573820783851694   T   T   T
  3.8340380237950304  4.8319692145357793 19.0084831543319233   T   T   T
  1.2432802037026500  6.8588406199338579 20.5901407963441727   T   T   T
  3.4664155156011809  7.4163378193015532 19.2962790021476565   T   T   T
  2.2878019967205034  5.6455787261017889 22.7776737570096337   T   T   T
  4.7263367725218188  6.9296880962480447 22.9129238998567288   T   T   T
  3.8014388285551783  6.5647919429662984 22.9703660359491693   T   T   T
  2.3882015746995511  4.6685967774291033 22.9218298388525774   T   T   T
  3.7373873653629164  4.8214874270666011  8.0000000000000000   F   F   F
  3.5428254414230036  5.7627092243419362  8.0158744918591047   F   F   F
  4.3147220498729837  7.8805540748890017  8.0308754104330866   F   F   F

Metal reference: O-a-SiO2(0001)/fcc(111)_sqrt13/Ru E_tot= -346.90422298 eV
 D3-zero damping= -13.455925 eV, D3-BJ damping= -16.3495463 eV
Ru
 1.0000000000000000
     9.6131018524371505    0.0000000000000000    0.0000000000000000
    -4.8065509262185726    8.3251904133778201    0.0000000000000000
     0.0000000000000013    0.0000000000000022   20.5497769047013250
  39
Cartesian
  0.0000826513396410  0.0000611627174696  8.1577662162144566
  2.5864426983151581  0.6384919669851078  8.1644494024803524
  7.7666900551685263  1.9205916063303354  8.1645047124865808
  0.7398747010818469  2.5588655681741841  8.1644977123994416
  3.3302111474177933  3.2041027686035490  8.1630370905908745
 -1.1099929157854205  4.4863543331104383  8.1627265064661483
  1.4762738425757496  5.1206987502797512  8.1626949740599883
  4.0663676232988166  5.7659368205456332  8.1644395513534853
 -0.3662209267738910  7.0432288367882947  8.1626890527510003
  2.2206039948119449  7.6864853264218604  8.1643858015191526
  8.1360317027188032  0.4271903432608939 10.2746743935190779
  1.1085874662729851  1.0655906280386673 10.2747348746579643
  6.2836480163010506  2.3478291207642972 10.2748597935757466
 -0.7411076848681556  2.9905283871419410 10.2743757365935782
  1.8462439296685527  3.6285766108600050 10.2746995680246602
  0.0000092103435196  5.5501224084072858 10.2748492021362381
  2.5873297237009507  6.1881746065173511 10.2742665790831733
  0.7410253199511938  8.1097879823209471 10.2747015706735301
 -3.3301026759545764  7.8963175169299920 12.3862488169836684
 -0.3667610186832277  1.4930290600322220 12.3862783903154359
  2.2200946156308454  2.1365690988161057 12.3849307582981201
  7.3925273384519388  3.4136908610763674 12.3850539492385359
  0.3663852708824048  4.0570565152918512 12.3862574059209170
  2.9606626539991705  4.6951595896647476 12.3849340642501851
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 -1.4762506923497141  5.9794798618487572 12.3863389250924634
  1.1099098245888284  6.6139431956721468 12.3861979316555466
  3.6969435574140115  7.2609187643257389 12.3862372972196848
  6.6528829488256411  0.8542927511143853 12.3849945534322305
  5.1731987450609838  1.2819555957198334  8.1629580373446178
  5.9163683213205189  3.8390617187169647  8.1630518314664844
 -2.9604362335347179  6.4050927668609061  8.1644481171396812
 -1.8460465710481371  7.4716882974048247 10.2743287363126345
  3.6980597916709383  1.7094967820510352 10.2747952295507829
  4.4380922174913771  4.2679027394400739 10.2748674454067022
 -2.5870354427028053  4.9120780552207295 10.2747304225034313
  5.1751840484890703  6.8323223443902217 10.2747250526018128
  4.0666442603362505  0.2163944678194401 12.3849581777753475
  4.8067571678889465  2.7750218830689124 12.3915656006390620
  5.5469711059246167  5.3342786720518474 12.3848826350172825

Interface: 3O-g-Al2O3(110)/fcc(100)_3x3/Au E_tot= -837.53617179 eV
 D3-zero damping= -36.6757481 eV, D3-BJ damping= -40.9310011 eV
 O Al  O Al  O Al  O Au
 1.0000000000000000
     8.6962551314100036    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6962551314100036    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.7575030025607248
  18  12  24  16  12   8   3  45
Selective dynamics
Cartesian
  3.5310462835323402  7.8063656642957868 10.9423958550990683   F   F   F
  7.9821910815116253  5.3364790554512664  9.3854545373318246   F   F   F
  3.5321145935263831  7.4284524359483344  8.0000187449185951   F   F   F
  3.6344616810693871  3.3543474123970207  8.1990827428381010   F   F   F
  7.8802281380900832  1.2624174968523383  9.5845317789161761   F   F   F
  3.6271666011832795  3.1554369468752417 10.8220669229527680   F   F   F
  0.7083960021202884  3.3544316428158409  8.1993257849376420   F   F   F
  5.1588358854150016  1.2623087994643727  9.5846030099037201   F   F   F
  0.7160901952006844  3.1553045949744871 10.8217845066302907   F   F   F
  0.8118413287580194  7.8064783860657743 10.9423584978630899   F   F   F
  5.0560005793416138  5.3365720443687925  9.3853700880230981   F   F   F
  0.8106713855975951  7.4281840563327339  8.0000000000000000   F   F   F
  6.5192511574305740  7.6188020475596341 10.9172067463060039   F   F   F
  6.5192057185729801  7.7314754794541836  8.0327436308783255   F   F   F
  2.1717681959075095  0.9592602948928505  9.5519775531218265   F   F   F
  2.1716499835923124  5.5649932499595769  9.4220834377914784   F   F   F
  6.5193476785207736  3.1257350510745350  8.1626394660302282   F   F   F
  6.5194342443598448  3.2340497157512256 10.8301543211852653   F   F   F
  0.6529590787385497  5.3305977833481926  8.0560139425344559   F   F   F
  5.0011162574095147  3.3603749684517115  9.5285274732362595   F   F   F
  0.6828365157980596  1.1907892444500303 10.9191009939757393   F   F   F
  8.0377282287004821  3.3603184787138018  9.5284873332419124   F   F   F
  3.6599190301032727  1.1908533309865517 10.9192047381793671   F   F   F
  3.6895912828186770  5.3305164729746144  8.0559839586400095   F   F   F
  6.5190859549397233  1.0905682195122306  8.1168144920444938   F   F   F
  6.5194715415604199  1.0897006865345162 10.8835529458276739   F   F   F
  6.5191569704862573  6.4821600504198278  9.4463612987341499   F   F   F
  2.1718420852423406  7.6002031203212406  9.4677862360962415   F   F   F
  2.1714813503303882  2.2087144238198260  8.1383270166926529   F   F   F
  2.1715979796152878  4.3361109845775054 10.8469192662674665   F   F   F
  3.5175709192046765  7.9163707453137286 16.4087261398969311   T   T   T
  7.9541330878762704  5.2469604951817148 14.9033050730958223   T   T   T
  3.5321145935263831  7.4284524359483344 13.5580397357678457   F   F   F
  7.9747256490413179  5.5352448492610788 12.3205669558782276   F   F   F
  7.8788760809173155  0.8845355344362547 12.2001224306209899   F   F   F
  3.6344616810693871  3.3543474123970207 13.7571037336873516   F   F   F
  7.8047992768686987  1.3569860895337114 15.0581927777754689   T   T   T
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3.5729180014614430	3.0522229032886998	16.2410028273929861	T	T	T
5.1596266770472559	0.8844520387713608	12.2001609218852387	F	F	F
0.7083960021202884	3.3544316428158409	13.7573467757868890	F	F	F
5.2225966790136464	1.3410257043232603	15.0922566295736136	T	T	T
0.7141269532067561	2.9966306829437408	16.2859874083428373	T	T	T
0.9333420082166326	7.8428229317239717	16.3258729347413194	T	T	T
5.0812957494374702	5.2428009721564832	14.8926961362191594	T	T	T
0.8106713855975951	7.4281840563327339	13.5580209908492506	F	F	F
5.0637449340171754	5.5351531724033096	12.3204488991888113	F	F	F
6.3846873508978677	7.3882163145496405	16.4390929885814145	T	T	T
6.5192057185729801	7.7314754794541836	13.5907646217275762	F	F	F
2.1714213028133433	1.0719992175167494	12.2256103096605884	F	F	F
2.1844408818168288	0.9626801716008133	15.0047955214896529	T	T	T
2.1822734804381527	5.5192964833342844	14.8735900516339310	T	T	T
2.1715094718585832	5.4566459574430537	12.3122395822918413	F	F	F
6.5193476785207736	3.1257350510745350	13.7206604568794788	F	F	F
6.5133973127480438	3.2709190559648786	16.3702417116685801	T	T	T
0.6529590787385497	5.3305977833481926	13.6140349333837065	F	F	F
5.0307943322257458	7.4998334412120302	12.2234202596149473	F	F	F
5.0091495691841379	3.3414749572726241	15.0222271892101276	T	T	T
0.6032584833165610	1.0554820614553988	16.3025552344280982	T	T	T
8.0174334829004543	3.3327597212651598	15.0325675148130014	T	T	T
3.6403717000375253	1.1524847606946789	16.2771825447021072	T	T	T
3.6895912828186770	5.3305164729746144	13.6140049494892601	F	F	F
8.0078230000662902	7.4998959336838711	12.2233730105456431	F	F	F
6.5190859549397233	1.0905682195122306	13.6748354828937444	F	F	F
6.5121029961267407	1.3112986490899867	16.5158411046182607	T	T	T
6.5103229371311819	6.3777136054475907	14.9579213761227443	T	T	T
2.2054625124647464	7.5623570431472933	15.0256019253541702	T	T	T
2.1713481796615515	7.6013207773936822	12.2590327337071869	F	F	F
2.1714813503303882	2.2087144238198260	13.6963480075419035	F	F	F
2.1239324724242534	4.1321848850871996	16.1421704223604046	T	T	T
6.5192328367062737	4.3545065208273153	12.2955930440659955	F	F	F
3.4575241846744849	7.1894864137718919	18.8105815560189775	T	T	T
7.8008520964446744	5.5403115265671872	17.9350376061403658	T	T	T
7.8954574720714055	0.6914635786402337	17.4956254781181606	T	T	T
3.3800250074049214	3.2514648664824439	18.9963446173336443	T	T	T
5.0057900369305539	1.1023482127136874	17.5959184270933093	T	T	T
0.4854201173264910	3.4909340899782513	19.1251661938921842	T	T	T
0.6356983571312960	7.2648907133402361	18.8267651120755062	T	T	T
4.9409335901293918	5.3970434345058287	17.8728441506036049	T	T	T
6.3014605291061407	7.6039623692304010	18.9506795702654038	T	T	T
2.0746442877323439	1.0536536491651762	17.7012420496124925	T	T	T
2.0377373823336828	5.2122251512799247	17.5469105344694292	T	T	T
6.1898701642561722	3.2857516203393553	19.1362714639099742	T	T	T
0.6799518390849699	5.2985007594224722	18.7652374983202357	T	T	T
4.9555096062621047	7.2783977629424736	17.7076734145372328	T	T	T
3.3823066597795779	5.1987446599753344	18.7676529016187850	T	T	T
7.7529533726182311	7.5179862730489866	17.8182429504478534	T	T	T
4.8295490540532162	2.1866809768508362	18.9974628693212715	T	T	T
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1.8165935967418192	2.3280073085996129	18.9756621704176389	T	T	T
6.4488230982590364	4.4241879054236932	17.8124307973750717	T	T	T
1.6776435604577320	1.4123043475987946	20.5171054521825411	T	T	T
4.6401902289191925	1.2172770175605809	20.4640549126798348	T	T	T
2.1000753885115104	5.3012419567867717	20.1219201980992644	T	T	T
0.3749386861848727	-0.3537322756530419	21.1188897118041403	T	T	T
2.2912148711649323	1.2151774097927819	23.5752320856761770	T	T	T
0.7401096905611894	-0.1855357503102405	25.5954929365222910	T	T	T
0.0551430175211006	2.8506428838612159	21.2275149435576580	T	T	T
2.0984248203528058	4.1545045099963076	23.5678758340436652	T	T	T
0.7326763276992637	2.7087565488694132	25.6084748569218519	T	T	T
0.5150984857903348	5.6267899881651759	21.6410676397234845	T	T	T

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  2.1264310114315879  7.0797050618594604 23.5155303741806918   T   T   T
  0.7085541787015340  5.6411198676229706 25.5760429427991909   T   T   T
  3.2266972422648679 -0.3926150610724468 21.2846029984808673   T   T   T
  5.1846047795704093  1.3956351363146751 23.6450581311313108   T   T   T
  3.6627729077406355 -0.1852186381569040 25.6229407437485897   T   T   T
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  5.0724430896892425  4.3133975543731120 23.6924447941292478   T   T   T
  3.6254874922402740  2.7683704907963107 25.6521907374519813   T   T   T
  3.8390247773036932  5.6460314913295866 21.5619486229183366   T   T   T
  5.0572095509113755  7.2821339546527195 23.4185883984636476   T   T   T
  3.5921064483773386  5.6801494927897052 25.6482116934607731   T   T   T
  6.6207871899968618  0.9632527216237778 21.2719404348441827   T   T   T
  8.1909175322116674  1.2863879776671037 23.4560390479411289   T   T   T
  6.5763928078567426 -0.1219364772512946 25.5571102499734302   T   T   T
  6.3008656427159568  4.0791698968204262 21.2365843680480317   T   T   T
  7.8829155303825447  4.1755921643940797 23.5868749372236088   T   T   T
  6.5670897399748966  2.7781178767204948 25.6664359975451752   T   T   T
  6.4396713657532949  6.9030642112197542 20.9541986271833700   T   T   T
  7.8438413986129314  7.1146172692638938 23.4572234738359491   T   T   T
  6.5122886344373034  5.7202512414753581 25.6358307746796932   T   T   T
  2.1966982619890021  1.2826399497699768 27.6699172506394468   T   T   T
  0.7308930085094504 -0.1569511524725347 29.7583975418574553   T   T   T
  2.1551631270733935  4.1802742737804177 27.6817898101408950   T   T   T
  0.7312214005108142  2.7308715926598954 29.7611290377474944   T   T   T
  2.1620775575256901  7.0959688135520542 27.6847125599998272   T   T   T
  0.7234463842949375  5.6437565972726285 29.7621804240234376   T   T   T
  5.1011029549765894  1.2962647259877458 27.6639819859745515   T   T   T
  3.6296248843158163 -0.1491376736066433 29.7633727061882496   T   T   T
  5.0737878921789950  4.2226486195277015 27.6825324886036164   T   T   T
  3.6344047144780340  2.7441224750442625 29.7472498236601020   T   T   T
  5.0841229223338260  7.1221655587658450 27.6953982653105406   T   T   T
  3.6138962897932161  5.6434630120411553 29.7488476081857911   T   T   T
  7.9818289784580845  1.2904112920864674 27.6808145781589658   T   T   T
  6.5350284154384424 -0.1423478285276214 29.7733183397239962   T   T   T
  7.9942237669140308  4.2096218441191571 27.6782918425229205   T   T   T
  6.5307024591454992  2.7545407254922578 29.7461612434452363   T   T   T
  7.9763018286734306  7.1040821442864557 27.6665585726790368   T   T   T
  6.5265072143055169  5.6540100560717788 29.7526364715991889   T   T   T

Oxide reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Au E_tot= -703.49104715 eV
 D3-zero damping= -9.8752019 eV, D3-BJ damping= -15.0029797 eV
 O Al  O Al  O Al  H  O  H  O  H  O  H
 1.0000000000000000
     8.6962551314100036    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6962551314100036    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.2904852797336304
  18  12  24  16  12   8   1   1   1   1   1   1   3
Selective dynamics
Cartesian
  3.5310462835323402  7.8063656642957868 10.9423958550990683   F   F   F
  7.9821910815116253  5.3364790554512664  9.3854545373318246   F   F   F
  3.5321145935263831  7.4284524359483344  8.0000187449185951   F   F   F
  3.6344616810693871  3.3543474123970207  8.1990827428381010   F   F   F
  7.8802281380900832  1.2624174968523383  9.5845317789161761   F   F   F
  3.6271666011832795  3.1554369468752417 10.8220669229527680   F   F   F
  0.7083960021202884  3.3544316428158409  8.1993257849376420   F   F   F
  5.1588358854150016  1.2623087994643727  9.5846030099037201   F   F   F
  0.7160901952006844  3.1553045949744871 10.8217845066302907   F   F   F
  0.8118413287580194  7.8064783860657743 10.9423584978630899   F   F   F
  5.0560005793416138  5.3365720443687925  9.3853700880230981   F   F   F
  0.8106713855975951  7.4281840563327339  8.0000000000000000   F   F   F
  6.5192511574305740  7.6188020475596341 10.9172067463060039   F   F   F
  6.5192057185729801  7.7314754794541836  8.0327436308783255   F   F   F
```

2.1717681959075095	0.9592602948928505	9.5519775531218265	F	F	F
2.1716499835923124	5.5649932499595769	9.4220834377914784	F	F	F
6.5193476785207736	3.1257350510745350	8.1626394660302282	F	F	F
6.5194342443598448	3.2340497157512256	10.8301543211852653	F	F	F
0.6529590787385497	5.3305977833481926	8.0560139425344559	F	F	F
5.0011162574095147	3.3603749684517115	9.5285274732362595	F	F	F
0.6828365157980596	1.1907892444500303	10.9191009939757393	F	F	F
8.0377282287004821	3.3603184787138018	9.5284873332419124	F	F	F
3.6599190301032727	1.1908533309865517	10.9192047381793671	F	F	F
3.6895912828186770	5.3305164729746144	8.0559839586400095	F	F	F
6.5190859549397233	1.0905682195122306	8.1168144920444938	F	F	F
6.5194715415604199	1.0897006865345162	10.8835529458276739	F	F	F
6.5191569704862573	6.4821600504198278	9.4463612987341499	F	F	F
2.1718420852423406	7.6002031203212406	9.4677862360962415	F	F	F
2.1714813503303882	2.2087144238198260	8.1383270166926529	F	F	F
2.1715979796152878	4.3361109845775054	10.8469192662674665	F	F	F
3.5077148981103519	7.8673261767863627	16.4360782576662885	T	T	T
7.9642161738384889	5.2454269449114133	14.9030138870892941	T	T	T
3.5321145935263831	7.4284524359483344	13.5580397357678457	F	F	F
7.9747256490413179	5.5352448492610788	12.3205669558782276	F	F	F
7.8788760809173155	0.8845355344362547	12.2001224306209899	F	F	F
3.6344616810693871	3.3543474123970207	13.7571037336873516	F	F	F
7.8013065387654716	1.3686490416508483	15.0629117143783766	T	T	T
3.5933692032591384	3.0805463579434935	16.2863686604350875	T	T	T
5.1596266770472559	0.8844520387713608	12.2001609218852387	F	F	F
0.7083960021202884	3.3544316428158409	13.7573467757868890	F	F	F
5.2227875547515952	1.3495409545497274	15.1179680448220832	T	T	T
0.6931420120285092	3.0142703510982489	16.2816929984747638	T	T	T
0.9257592041535827	7.8646656713898171	16.3102847058026725	T	T	T
5.0702515709955929	5.2456982429838925	14.9041045628395903	T	T	T
0.8106713855975951	7.4281840563327339	13.5580209908492506	F	F	F
5.0637449340171754	5.5351531724033096	12.3204488991888113	F	F	F
6.4228888106852002	7.2806277026213113	16.4528858529513187	T	T	T
6.5192057185729801	7.7314754794541836	13.5907646217275762	F	F	F
2.1714213028133433	1.0719992175167494	12.2256103096605884	F	F	F
2.2101060917167064	0.9767854012704512	15.0247161270929919	T	T	T
2.1733713063114952	5.5221698740836818	14.8940060099383302	T	T	T
2.1715094718585832	5.4566459574430537	12.3122395822918413	F	F	F
6.5193476785207736	3.1257350510745350	13.7206604568794788	F	F	F
6.5135927786272125	3.3036216213025487	16.3603527746624202	T	T	T
0.6529590787385497	5.3305977833481926	13.6140349333837065	F	F	F
5.0307943322257458	7.4998334412120302	12.2234202596149473	F	F	F
5.0128951566362492	3.3502005896338511	15.0167788864209406	T	T	T
0.6067337289474773	1.0889499929267308	16.2836028970265936	T	T	T
8.0131620083018031	3.3433205024370527	15.0146657526414380	T	T	T
3.6601492960409479	1.1824447737230623	16.3097306917221623	T	T	T
3.6895912828186770	5.3305164729746144	13.6140049494892601	F	F	F
8.0078230000662902	7.4998959336838711	12.2233730105456431	F	F	F
6.5190859549397233	1.0905682195122306	13.6748354828937444	F	F	F
6.5248892880682225	1.3729361726103766	16.5315923503913176	T	T	T
6.5182471010917027	6.3570067143028295	14.9230834775378600	T	T	T
2.1980328978556498	7.5614115275417690	15.0053119036196634	T	T	T
2.1713481796615515	7.6013207773936822	12.2590327337071869	F	F	F
2.1714813503303882	2.2087144238198260	13.6963480075419035	F	F	F
2.1157842185550635	4.1163909788609656	16.1222609818245282	T	T	T
6.5192328367062737	4.3545065208273153	12.2955930440659955	F	F	F
3.5504363103718712	7.5311054548402447	18.8526787672881966	T	T	T
7.8510550827613041	5.4836645127828376	18.0088145501569876	T	T	T
7.9071682091747508	0.6916384988889046	17.4882196015320375	T	T	T
3.4837546725222444	3.0159701739131997	19.2245556780750455	T	T	T
5.0372479912968675	1.0859142559810775	17.6142598668674744	T	T	T
0.6131492339960690	3.4678116272256685	19.2667948061326264	T	T	T
0.7197304368670892	7.2287179546403406	18.7862869213551953	T	T	T

```
  4.9424492248498915  5.3936040397421587 18.0066915308202162   T   T   T
  6.3449999559438073  7.5814087798450016 18.9073902853415632   T   T   T
  2.0688341554526803  1.0919150573193452 17.6845164287738079   T   T   T
  2.1416692555758381  5.1052874013094049 17.6077446942377200   T   T   T
  6.3546175947686994  3.1837995000771913 19.1273514335015129   T   T   T
  0.7711409823904974  5.3596887056855209 18.7823159794707557   T   T   T
  4.9862359108970109  7.2745424186164351 17.6496612767615453   T   T   T
  3.4699513888479521  4.7656481673164564 18.7595959881158336   T   T   T
  7.8320663107064679  7.4997788514716248 17.7792465047948589   T   T   T
  5.0487719750407747  2.0417216842676735 19.1557332022997784   T   T   T
  2.0799881696492641  7.9168141118829185 17.7951842983817485   T   T   T
  1.8842798890551113  2.1320486235135752 19.1760619615825085   T   T   T
  6.4685927162362766  4.3882777931738897 17.8709382564248003   T   T   T
  8.3689284824786050  3.1454274640174624 19.3081366653058346   T   T   T
  1.7179101290170098  1.0662351029276627 20.5213103937344243   T   T   T
  1.1859118134296658  0.2572502267306536 20.4334656650068780   T   T   T
  5.0069188386033989  0.7717697540640192 20.3731661991090363   T   T   T
  4.7777711934895066  0.9603732503325483 21.2947628677655452   T   T   T
  2.2990882332069109  5.3525429310007011 20.0680838994126489   T   T   T
  2.2217020261026938  4.8308154243570813 20.8828049950044523   T   T   T
  3.7428611223722239  8.0313212068473465 19.6786784526093435   T   T   T
  6.1555542948842765  8.2291774921181879 19.6227175954934872   T   T   T

Metal reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Au E_tot= -159.69647968 eV
 D3-zero damping= -22.8620021 eV, D3-BJ damping= -22.7531399 eV
Au
 1.0000000000000000
     8.6962551314100036    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6962551314100036    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0004513041461060 -0.0004521478249009  7.6902785096333410
  1.4488052971537153  1.4488046968689963  9.7642512387830838
 -0.0003264515018972 -0.0003264029968842 11.8274829358139009
  1.4486340926622530  1.4486343530167267 13.8909255075381193
 -0.0004930902193350 -0.0004923822173292 15.9656612773392474
 -0.0004513617372237  2.8982995115579913  7.6902784933907125
  1.4488053392557636  4.3475563251389504  9.7642512352211579
 -0.0003264279439596  2.8984253026937727 11.8274829059435724
  1.4486340295025690  4.3473860924052010 13.8909254347227034
 -0.0004930904740366  2.8982594410924225 15.9656613404989258
 -0.0004512985775402  5.7970511990889966  7.6902784933907169
  1.4488051905304458  7.2463081367532558  9.7642511955601989
 -0.0003264517565989  5.7971770179431026 11.8274828729790009
  1.4486341579076387  7.2461378028752028 13.8909253911364345
 -0.0004931029000373  5.7970111515624252 15.9656613056681724
  2.8983003716717768 -0.0004522366947585  7.6902784933907125
  4.3475570286456895  1.4488047260715566  9.7642511678716559
  2.8984253092507504 -0.0003264029968842 11.8274828335121409
  4.3473858347452996  1.4486343530167267 13.8909254190744971
  2.8982586970342292 -0.0004922693775838 15.9656612935818725
  2.8983003720291745  2.8982994886189934  7.6902785070146065
  4.3475570286456895  4.3475563970806954  9.7642511736949427
  2.8984253092507504  2.8984252443134291 11.8274828892216242
  4.3473857400521627  4.3473860924052010 13.8909253687918497
  2.8982586467515858  2.8982594675933426 15.9656614191104769
  2.8983003557865490  5.7970511990889966  7.6902785482205562
  4.3475569832005041  7.2463081367532558  9.7642510417941732
  2.8984252201261906  5.7971770682257473 11.8274828112504462
  4.3473857402973612  7.2461377478132150 13.8909253687918497
  2.8982586364932907  5.7970111515624252 15.9656613955609075
  5.7970521511573496 -0.0004521751685466  7.6902784933907125
```

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  7.2463087391156904  1.4488046968689963  9.7642512352211579
  5.7971769166651548 -0.0003264029968842 11.8274828226963553
  7.2461374633196218  1.4486343819351910 13.8909254347227034
  5.7970103342825920 -0.0004924473054639 15.9656612935818725
  5.7970521771922900  2.8982995115579913  7.6902784933907125
  7.2463087731557092  4.3475564365415504  9.7642512122821632
  5.7971769811335330  2.8984252782705524 11.8274828744101548
  7.2461374004847201  4.3473860634867476 13.8909253844400613
  5.7970103077816715  2.8982593263242200 15.9656613276218913
  5.7970521223624498  5.7970511990889966  7.6902784766687624
  7.2463086840537079  7.2463080967289084  9.7642511933378948
  5.7971769182986375  5.7971770682257473 11.8274827578860258
  7.2461374001599355  7.2461378028752010 13.8909253681974363
  5.7970102801833221  5.7970109736345403 15.9656613029665326

Interface: 3O-g-Al2O3(110)/fcc(100)_3x3/Ag E_tot= -813.08629516 eV
 D3-zero damping= -30.6195029 eV, D3-BJ damping= -38.9291165 eV
 O Al  O Al  O Al  O Ag
 1.0000000000000000
     8.6415811558500017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6415811558500017    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.3375309279805094
  18  12  24  16  12   8   3  45
Selective dynamics
Cartesian
  3.5088463439848243  7.7572864872140848 10.9423958550990701   F   F   F
  7.9320064775055261  5.3029282314419337  9.3854545373318263   F   F   F
  3.5099079374378253  7.3817492262569910  8.0000187449185969   F   F   F
  3.6116115615499145  3.3332583912409213  8.1990827428381028   F   F   F
  7.8306845823734390  1.2544805881109971  9.5845317789161779   F   F   F
  3.6043623463507752  3.1355984899868905 10.8220669229527697   F   F   F
  0.7039422659865778  3.3333420920970971  8.1993257849376437   F   F   F
  5.1264019166715498  1.2543725741112535  9.5846030099037218   F   F   F
  0.7115880851269187  3.1354669701919655 10.8217845066302925   F   F   F
  0.8067372244859640  7.7573985002942738 10.9423584978630917   F   F   F
  5.0242131434937596  5.3030206357315102  9.3853700880230999   F   F   F
  0.8055746368415397  7.3814825339631538  8.0000000000000018   F   F   F
  6.4782641609516567  7.5709020962989797 10.9172067463060056   F   F   F
  6.4782190077713988  7.6828671422999957  8.0327436308783273   F   F   F
  2.1581141345361776  0.9532293570781101  9.5519775531218283   F   F   F
  2.1579966654302276  5.5300057409292931  9.4220834377914802   F   F   F
  6.4783600752068864  3.1060833321211403  8.1626394660302299   F   F   F
  6.4784460968003605  3.2137170147843279 10.8301543211852671   F   F   F
  0.6488538784916427  5.2970839353155723  8.0560139425344577   F   F   F
  4.9696738832037806  3.3392480516212739  9.5285274732362613   F   F   F
  0.6785434739757958  1.1833026676345666 10.9191009939757411   F   F   F
  7.9871944586933639  3.3391919170383710  9.5284873332419142   F   F   F
  3.6369088584167617  1.1833663512544670 10.9192047381793689   F   F   F
  3.6663945595653988  5.2970031361461061  8.0559839586400113   F   F   F
  6.4780999971006361  1.0837117394206146  8.1168144920444956   F   F   F
  6.4784831595107777  1.0828496606845370 10.8835529458276756   F   F   F
  6.4781705661673703  6.4414062483731760  9.4463612987341516   F   F   F
  2.1581875593234963  7.5524201018411805  9.4677862360962433   F   F   F
  2.1578290923776358  2.1948280788814425  8.1383270166926547   F   F   F
  2.1579449884059114  4.3088495458991538 10.8469192662674683   F   F   F
  3.4988874632174327  7.8488611187475890 16.4162821286171727   T   T   T
  7.9066706191283744  5.2252689843097375 14.9089775529688726   T   T   T
  3.5099079374378253  7.3817492262569910 13.5580397357678475   F   F   F
  7.9245879807410207  5.5004443705453570 12.3205669558782294   F   F   F
  7.8293410256804412  0.8789743965141341 12.2001224306209917   F   F   F
  3.6116115615499145  3.3332583912409213 13.7571037336873534   F   F   F
  7.7696731083609132  1.3357191539835080 15.0636682290348087   T   T   T
  3.5793244992649789  3.0334799028133150 16.2588217719100037   T   T   T
```

5.1271877365404732	0.8788914257924338	12.2001609218852405	F	F	F
0.7039422659865778	3.3333420920970971	13.7573467757868908	F	F	F
5.1931189770874653	1.3186054800861333	15.1096711666828263	T	T	T
0.7271676951760068	2.9986901442387044	16.2835666129276468	T	T	T
0.9154317182658170	7.7813263000458228	16.3537409834730703	T	T	T
5.0475670711335505	5.2224967923008361	14.9063629982137211	T	T	T
0.8055746368415397	7.3814825339631538	13.5580209908492524	F	F	F
5.0319088088597432	5.5003532700665243	12.3204488991888130	F	F	F
6.3899581265853058	7.3914945833463346	16.4478320154147752	T	T	T
6.4782190077713988	7.6828671422999957	13.5907646217275779	F	F	F
2.1577694223836081	1.0652594820635937	12.2256103096605901	F	F	F
2.1709273763359906	0.9506703016105400	15.0098146293301848	T	T	T
2.1677009870602801	5.4885660709874839	14.8718014699803280	T	T	T
2.1578570371037791	5.4223396355598270	12.3122395822918431	F	F	F
6.4783600752068864	3.1060833321211403	13.7206604568794805	F	F	F
6.4861145404344347	3.2464970217880307	16.3604340436056859	T	T	T
0.6488538784916427	5.2970839353155723	13.6140349333837083	F	F	F
4.9991653698492824	7.4526814540551847	12.2234202596149490	F	F	F
4.9908123421748156	3.3228263794628816	15.0286508941297523	T	T	T
0.6273934169740876	1.0696618352038423	16.3142296657078667	T	T	T
7.9730056355957037	3.3151983566734637	15.0367261153830380	T	T	T
3.6263925561808863	1.1387903729693705	16.2918801747162263	T	T	T
3.6663945595653988	5.2970031361461061	13.6140049494892619	F	F	F
7.9574772463621377	7.4527435536324029	12.2233730105456448	F	F	F
6.4780999971006361	1.0837117394206146	13.6748354828937462	F	F	F
6.4966418515438882	1.2691198633654408	16.5159925649655079	T	T	T
6.4718233797072626	6.3584662158312826	14.9685630334047168	T	T	T
2.1848769403115460	7.5111054166721880	15.0279228748413161	T	T	T
2.1576967589622811	7.5535307321239822	12.2590327337071887	F	F	F
2.1578290923776358	2.1948280788814425	13.6963480075419053	F	F	F
2.1385820149601007	4.1169346352164613	16.1382178966612102	T	T	T
6.4782459554110563	4.3271294281020038	12.2955930440659973	F	F	F
3.5202845148862916	7.2113517583294833	18.8605199604894374	T	T	T
7.8251395924073810	5.5118422442432280	17.9135835448456007	T	T	T
7.8901773739093324	0.7222157799732752	17.5254611192922525	T	T	T
3.4484037144025619	3.2244220575233697	19.0230179920491089	T	T	T
4.9974591558180350	1.0275278924075464	17.6338954097472289	T	T	T
0.5512069332137454	3.4575984872955581	19.1523104286038404	T	T	T
0.7045400019680172	7.2176049906082742	18.8561759846494397	T	T	T
5.0014512922305014	5.4122604865929658	17.9318909661531869	T	T	T
6.3873309965270710	7.6007687374920438	19.0078289276617127	T	T	T
2.1007707231686972	1.0541210824676954	17.6849417743937209	T	T	T
2.1080332133520288	5.2150690627516489	17.5319450106015751	T	T	T
6.2628476911107160	3.2275128593811488	19.1004445198484234	T	T	T
0.7489080381794669	5.2295310454462411	18.7532207907779771	T	T	T
5.0152320592140303	7.3201258247284313	17.7616481438552327	T	T	T
3.4278955345261846	5.1622193018851492	18.7656525319396579	T	T	T
7.8036468385508853	7.4744796184146276	17.7993263830263579	T	T	T
4.8942227662610209	2.1461226890607716	19.0398475306640016	T	T	T
2.1236670015817847	7.7800153324161050	17.8152699823681928	T	T	T
1.8652311345313848	2.3021241533616643	18.9912381154517611	T	T	T
6.4763635118093061	4.3877991512070880	17.8085907490271467	T	T	T
1.8774528232677581	1.3380009676070792	20.4943372954694958	T	T	T
4.8889958061111889	1.3646802636874000	20.6238481654174102	T	T	T
2.1436320985327950	5.2919184393113134	20.0945668040909418	T	T	T
0.7800828313018189	-0.5209856015031948	21.0695859486252246	T	T	T
1.8347292954789598	1.1981442606378214	23.4094951213615374	T	T	T
0.4825475391969193	-0.1836105805859621	25.5015381936482335	T	T	T
0.1426953210960791	2.6907555513202879	21.2969107670058051	T	T	T
1.8779993383636808	4.0927611205836616	23.5567304714351557	T	T	T
0.4497003535195006	2.6702337520977539	25.5329323009049887	T	T	T
0.4039112852586567	5.4624551830887773	21.5696775046002607	T	T	T
2.0040044349373654	7.0418967666403134	23.4360949919844828	T	T	T

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  0.4842208383717089  5.6161812393960506 25.5076740185507518   T   T   T
  3.6374757416823380 -0.4545841285330252 21.0851954603319491   T   T   T
  4.8014914056573410  1.1947260153058183 23.3985051520162841   T   T   T
  3.3837328214010483 -0.1901502430238960 25.4871337684289863   T   T   T
  3.3260773684618639  2.7714279687445953 21.6360882729687454   T   T   T
  4.8363985147364428  4.1063144913271818 23.6304892935829614   T   T   T
  3.3380813462941310  2.6431548776700153 25.5101015161386968   T   T   T
  3.6131539759847771  5.5200080704430086 21.6638312030967590   T   T   T
  4.9442795111926712  7.0387740262484977 23.4525304443349292   T   T   T
  3.3636379005540928  5.5936930875411282 25.5360718314684831   T   T   T
  6.9386399058843615  0.5048401571280144 20.7336055712909975   T   T   T
  7.6283110730815542  1.2866183425110258 23.3812781856327092   T   T   T
  6.2796325899780205 -0.1744026875609920 25.4946291203506590   T   T   T
  6.1837057068468235  3.6958672886370429 21.2627288750661982   T   T   T
  7.6470878882229636  4.1628300832360443 23.5468551622294768   T   T   T
  6.2404832355432722  2.6572466325548154 25.5487100838688193   T   T   T
  6.3038668733684675  6.4359894711194565 20.9189199580521645   T   T   T
  7.7401897570027689  7.1237904365018547 23.3351243664586185   T   T   T
  6.2744666850122632  5.6182308370164522 25.5622682625480948   T   T   T
  1.9208221847540785  1.2463654805362820 27.5690273543872912   T   T   T
  0.4892284548029200 -0.1801149992134320 29.6468858348074953   T   T   T
  1.9101320154069994  4.1269698136968014 27.5491325205272481   T   T   T
  0.4667214897160238  2.7076325375737258 29.6249762481603227   T   T   T
  1.9294707291962931  7.0313884731078744 27.5661084965415775   T   T   T
  0.4842838177972200  5.5817427430647868 29.6127683551607568   T   T   T
  4.7952469130345214  1.2431641696008304 27.5749288972800279   T   T   T
  3.3715126596353762 -0.1933052926573930 29.6374845707949284   T   T   T
  4.7888989099854706  4.1294273258127934 27.5445014325768653   T   T   T
  3.3476905004464985  2.7001864891074696 29.6172020743463591   T   T   T
  4.8113502023467234  7.0352410163969994 27.5645456087383458   T   T   T
  3.3620315995598160  5.5707265065544025 29.6003496777924262   T   T   T
  7.6765243986689935  1.2504927404311026 27.5907697827752223   T   T   T
  6.2511263900953464 -0.1814897605560012 29.6431886511930855   T   T   T
  7.6833689524608344  4.1410629549123605 27.5619954559097806   T   T   T
  6.2271161145691973  2.7085620404814907 29.6176660408841244   T   T   T
  7.7039797824223255  7.0406006016210769 27.5822593079967078   T   T   T
  6.2406350814977909  5.5820300480506528 29.5990319792147361   T   T   T

Oxide reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Ag E_tot= -705.00860624 eV
 D3-zero damping= -10.0186695 eV, D3-BJ damping= -15.1868543 eV
 O Al  O Al  O Al  H  O  H  O  H  O  H
 1.0000000000000000
     8.6415811558500017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6415811558500017    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.2904852797336304
  18  12  24  16  12   8   1   1   1   1   1   1   3
Selective dynamics
Cartesian
  3.5088463439848243  7.7572864872140848 10.9423958550990683   F   F   F
  7.9320064775055261  5.3029282314419337  9.3854545373318246   F   F   F
  3.5099079374378253  7.3817492262569910  8.0000187449185951   F   F   F
  3.6116115615499145  3.3332583912409213  8.1990827428381010   F   F   F
  7.8306845823734390  1.2544805881109971  9.5845317789161761   F   F   F
  3.6043623463507752  3.1355984899868905 10.8220669229527680   F   F   F
  0.7039422659865778  3.3333420920970971  8.1993257849376420   F   F   F
  5.1264019166715498  1.2543725741112535  9.5846030099037201   F   F   F
  0.7115880851269187  3.1354669701919655 10.8217845066302907   F   F   F
  0.8067372244859640  7.7573985002942738 10.9423584978630899   F   F   F
  5.0242131434937596  5.3030206357315102  9.3853700880230981   F   F   F
  0.8055746368415397  7.3814825339631538  8.0000000000000000   F   F   F
  6.4782641609516567  7.5709020962989797 10.9172067463060039   F   F   F
  6.4782190077713988  7.6828671422999957  8.0327436308783255   F   F   F
  2.1581141345361776  0.9532293570781101  9.5519775531218265   F   F   F
```

2.1579966654302276	5.5300057409292931	9.4220834377914784	F	F	F
6.4783600752068864	3.1060833321211403	8.1626394660302282	F	F	F
6.4784460968003605	3.2137170147843279	10.8301543211852653	F	F	F
0.6488538784916427	5.2970839353155723	8.0560139425344559	F	F	F
4.9696738832037806	3.3392480516212739	9.5285274732362595	F	F	F
0.6785434739757958	1.1833026676345666	10.9191009939757393	F	F	F
7.9871944586933639	3.3391919170383710	9.5284873332419124	F	F	F
3.6369088584167617	1.1833663512544670	10.9192047381793671	F	F	F
3.6663945595653988	5.2970031361461061	8.0559839586400095	F	F	F
6.4780999971006361	1.0837117394206146	8.1168144920444938	F	F	F
6.4784831595107777	1.0828496606845370	10.8835529458276739	F	F	F
6.4781705661673703	6.4414062483731760	9.4463612987341499	F	F	F
2.1581875593234963	7.5524201018411805	9.4677862360962415	F	F	F
2.1578290923776358	2.1948280788814425	8.1383270166926529	F	F	F
2.1579449884059114	4.3088495458991538	10.8469192662674665	F	F	F
3.4862932914954246	7.8094727065154768	16.4457255281253865	T	T	T
7.9159993282220702	5.2208294262278416	14.9084779392472004	T	T	T
3.5099079374378253	7.3817492262569910	13.5580397357678457	F	F	F
7.9245879807410207	5.5004443705453570	12.3205669558782276	F	F	F
7.8293410256804412	0.8789743965141341	12.2001224306209899	F	F	F
3.6116115615499145	3.3332583912409213	13.7571037336873516	F	F	F
7.7589447698474228	1.3500072529847174	15.0656248587987065	T	T	T
3.5773135838896621	3.0640084272542758	16.2939004247333692	T	T	T
5.1271877365404732	0.8788914257924338	12.2001609218852387	F	F	F
0.7039422659865778	3.3333420920970971	13.7573467757868890	F	F	F
5.1853813468131964	1.3310237024893647	15.1224179539930930	T	T	T
0.6931808104091584	3.0064487959587129	16.2891000370182901	T	T	T
0.9067457389467153	7.7989881533694456	16.3315211460151204	T	T	T
5.0373812409557797	5.2216968959448664	14.9109554290277213	T	T	T
0.8055746368415397	7.3814825339631538	13.5580209908492506	F	F	F
5.0319088088597432	5.5003532700665243	12.3204488991888113	F	F	F
6.3932730290585917	7.2771856435514986	16.4502542743370022	T	T	T
6.4782190077713988	7.6828671422999957	13.5907646217275762	F	F	F
2.1577694223836081	1.0652594820635937	12.2256103096605884	F	F	F
2.1896492291124767	0.9629042064804898	15.0299143875005470	T	T	T
2.1603588458960057	5.4916839678104523	14.9001661917191779	T	T	T
2.1578570371037791	5.4223396355598270	12.3122395822918413	F	F	F
6.4783600752068864	3.1060833321211403	13.7206604568794788	F	F	F
6.4741180433472820	3.2759177152728776	16.3602016303461504	T	T	T
0.6488538784916427	5.2970839353155723	13.6140349333837065	F	F	F
4.9991653698492824	7.4526814540551847	12.2234202596149473	F	F	F
4.9839200813651301	3.3304671653866880	15.0231587985784500	T	T	T
0.6114277766284181	1.0898476481267090	16.2936015837792105	T	T	T
7.9639601279560859	3.3246255615686122	15.0203037593342525	T	T	T
3.6363255733917965	1.1714376672125979	16.3194178934983967	T	T	T
3.6663945595653988	5.2970031361461061	13.6140049494892601	F	F	F
7.9574772463621377	7.4527435536324029	12.2233730105456431	F	F	F
6.4780999971006361	1.0837117394206146	13.6748354828937444	F	F	F
6.4887855920267068	1.3415092047142074	16.5299570653815735	T	T	T
6.4777494104810858	6.3332814905116432	14.9308317190163056	T	T	T
2.1791497449127091	7.5106266193456239	15.0114631955312507	T	T	T
2.1576967589622811	7.5535307321239822	12.2590327337071869	F	F	F
2.1578290923776358	2.1948280788814425	13.6963480075419035	F	F	F
2.1098566384975932	4.1070895886643344	16.1409140534392606	T	T	T
6.4782459554110563	4.3271294281020038	12.2955930440659955	F	F	F
3.5439492136036690	7.4797330052175246	18.8719950791020779	T	T	T
7.8237183350456556	5.4546361093662030	17.9863114925198531	T	T	T
7.8747803026083441	0.7098842203325684	17.5062734062591652	T	T	T
3.4766751552392923	2.9989980991135781	19.2349875911759796	T	T	T
5.0117627461056600	1.0578588641381341	17.6267349728419731	T	T	T
0.6057958206203630	3.4444929476133415	19.2817538109130204	T	T	T
0.7263449944843906	7.1932140923815506	18.8203604220034073	T	T	T
4.9314592614336856	5.3677340851966173	18.0075325941910975	T	T	T

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  6.3377840475848837  7.5332556199730796 18.9164682512996052   T   T   T
  2.0696697868687655  1.0839273883220786 17.6872772303326897   T   T   T
  2.1427807686401130  5.0955865276835173 17.6262793943088347   T   T   T
  6.3455230457931240  3.1607891810032664 19.1310840320560693   T   T   T
  0.7730395685455396  5.3281057792776965 18.8062117685375974   T   T   T
  4.9739329510827757  7.2538082413826421 17.6631912472577888   T   T   T
  3.4674987646247466  4.7524580696822163 18.7817475140093606   T   T   T
  7.8151981857818944  7.4610882053992951 17.7714830169840994   T   T   T
  5.0369279504217550  2.0220183277098176 19.1666978766500478   T   T   T
  2.0787052545126135  7.8521007770217128 17.8068327242335585   T   T   T
  1.8773425615911776  2.1132737814933629 19.1851726020140134   T   T   T
  6.4449159240195897  4.3583218485071269 17.8656969178222340   T   T   T
  8.3028503918625365  3.1238029876976876 19.3131189553981777   T   T   T
  1.7163478952782085  1.0383593478103499 20.5230715526370844   T   T   T
  1.1930921830429650  0.2243484522929773 20.4213702018200181   T   T   T
  4.9940448258102093  0.7629774461207330 20.3934028840283972   T   T   T
  4.7595731571081199  0.9578972942800573 21.3122420407138087   T   T   T
  2.2948293804251527  5.3182236284245823 20.0965720386806375   T   T   T
  2.2175581431266975  4.7772308184583316 20.8988165605947707   T   T   T
  3.7325938450212806  7.9851160775248609 19.6963667423535433   T   T   T
  6.1594524644884929  8.1742311333547732 19.6394496945267960   T   T   T

Metal reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Ag E_tot= -131.36629926 eV
 D3-zero damping= -16.936569 eV, D3-BJ damping= -20.6475888 eV
Ag
 1.0000000000000000
     8.6415811558500017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.6415811558500017    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0001009703296095 -0.0001016700434123  7.7258836695138298
  1.4400307318692709  1.4400300732652214  9.7725647429041853
 -0.0003232964402609 -0.0003231635632294 11.8271512840411095
  1.4394458355100475  1.4394462067322227 13.8829579852519114
 -0.0010923489894180 -0.0010917178330178 15.9300414833092656
 -0.0001009941403956  2.8804254430159308  7.7258837052662743
  1.4400307132981172  4.3205571804376470  9.7725647886942788
 -0.0003232964402608  2.8802039086243814 11.8271512466221989
  1.4394458915001056  4.3199732401110573 13.8829578839549619
 -0.0010923811686901  2.8794353189071793 15.9300413867565762
 -0.0001009703296095  5.7609524949659372  7.7258836084044784
  1.4400307132981172  7.2010841822845135  9.7725649643636974
 -0.0003232594403030  5.7607309641475517 11.8271512840411095
  1.4394458355100475  7.2005002697604734 13.8829580412419666
 -0.0010923811686901  5.7599623708571830 15.9300412646431759
  2.8804260578096073 -0.0001016089340708  7.7258835957202558
  4.3205577100257004  1.4400300732652214  9.7725647565123026
  2.8802038114997974 -0.0003231806241809 11.8271513448518544
  4.3199728374772501  1.4394461507421645 13.8829579852519114
  2.8794346469705299 -0.0010917330428272 15.9300415014219006
  2.8804260578096073  2.8804254430159308  7.7258835928174348
  4.3205577100257004  4.3205571804376470  9.7725647886942788
  2.8802038163204817  2.8802038900532287 11.8271512280510471
  4.3199728136664639  4.3199732401110573 13.8829579852519114
  2.8794347029605878  2.8794353189071793 15.9300415574119558
  2.8804260578096073  5.7609524949659372  7.7258835754826460
  4.3205577100257004  7.2010842382745714  9.7725647370172517
  2.8802038114997974  5.7607309232758146 11.8271512466221989
  4.3199728696565227  7.2005002697604734 13.8829580412419666
  2.8794346843894352  5.7599623708571830 15.9300415400418842
  5.7609531001432535 -0.0001016700434112  7.7258835928174348
  7.2010847993946063  1.4400300732652214  9.7725647886942788
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  5.7607308393298959 -0.0003231635632294 11.8271513448518544
  7.2004998894272498  1.4394461098704272 13.8829580181737349
  5.7599616616219746 -0.0010917178330179 15.9300414256492964
  5.7609531224438379  2.8804254430159308  7.7258835531820598
  7.2010847993946063  4.3205571990087996  9.7725649260175373
  5.7607308393298959  2.8802038475150402 11.8271512280510471
  7.2004998656164636  4.3199732348714246 13.8829579852519114
  5.7599617176120343  2.8794353189071793 15.9300413203241078
  5.7609531426814442  5.7609524949659372  7.7258836142914085
  7.2010847619757010  7.2010841822845135  9.7725647429041853
  5.7607307665880105  5.7607309232758146 11.8271512840411095
  7.2004998894272498  7.2005002697604734 13.8829580460626527
  5.7599616616219746  5.7599623708571830 15.9300415014219006

Interface: 3O-g-Al2O3(110)/fcc(100)_3x3/Cu E_tot= -846.80077441 eV
 D3-zero damping= -32.7061407 eV, D3-BJ damping= -42.6907183 eV
 O Al  O Al  O Al  O Cu
 1.0000000000000000
     7.5713089101900026    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.5713089101900026    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.1757818884185767
  18  12  24  16  12   8   3  45
Selective dynamics
Cartesian
  3.0742706814383642  6.7965354071552930 10.9423958550990683   F   F   F
  6.9496160755450562  4.6461529487152262  9.3854545373318246   F   F   F
  3.0752007950165097  6.4675089756823914  8.0000187449185951   F   F   F
  3.1643082791158981  2.9204295489932952  8.1990827428381010   F   F   F
  6.8608430427428830  1.0991113643589845  9.5845317789161761   F   F   F
  3.1579568896376000  2.7472501105824416 10.8220669229527680   F   F   F
  0.6167580046523641  2.9205028833781403  8.1993257849376420   F   F   F
  4.4914896717292514  1.0990167280483447  9.5846030099037201   F   F   F
  0.6234568781037551  2.7471348797031352 10.8217845066302907   F   F   F
  0.7068216598067383  6.7966335472545181 10.9423584978630899   F   F   F
  4.4019571249731957  4.6462339086007374  9.3853700880230981   F   F   F
  0.7058030603129238  6.4672753136124310  8.0000000000000000   F   F   F
  5.6759218341858286  6.6332349909229507 10.9172067463060039   F   F   F
  5.6758822732918386  6.7313330050628108  8.0327436308783255   F   F   F
  1.8908285973753074  0.8351705312417778  9.5519775531218265   F   F   F
  1.8907256769869536  4.8451065823013115  9.4220834377914784   F   F   F
  5.6760058693227018  2.7213904474369603  8.1626394660302282   F   F   F
  5.6760812370181952  2.8156935438133313 10.8301543211852653   F   F   F
  0.5684923931206077  4.6410324770634208  8.0560139425344559   F   F   F
  4.3541726304528670  2.9256773813273207  9.5285274732362595   F   F   F
  0.5945048895347544  1.0367489316290468 10.9191009939757393   F   F   F
  6.9979689459477150  2.9256281990931861  9.5284873332419124   F   F   F
  3.1864724694090163  1.0368047279410977 10.9192047381793671   F   F   F
  3.2123063240941336  4.6409616849872153  8.0559839586400095   F   F   F
  5.6757780022636899  0.9494924830044873  8.1168144920444938   F   F   F
  5.6761137094586616  0.9487371739588352 10.8835529458276739   F   F   F
  5.6758398312500882  5.6436288270516490  9.4463612987341499   F   F   F
  1.8908929283971920  6.6170420180407037  9.4677862360962415   F   F   F
  1.8905788580977576  1.9229954669488631  8.1383270166926529   F   F   F
  1.8906804002363682  3.7751923370469673 10.8469192662674665   F   F   F
  3.1129356432315594  6.6160898070159746 16.6420835552923307   T   T   T
  6.9871037257955066  4.7079839114564930 15.0129569879139684   T   T   T
  3.0752007950165097  6.4675089756823914 13.5580397357678457   F   F   F
  6.9431163702665497  4.8192064301244377 12.3205669558782276   F   F   F
  6.8596658874772460  0.7701121542613976 12.2001224306209899   F   F   F
  3.1643082791158981  2.9204295489932952 13.7571037336873516   F   F   F
  6.8748160767194726  1.0163559116695260 15.1948947203670190   T   T   T
  3.1692683786682765  2.7897568834044102 16.5288755959286604   T   T   T
  4.4921781666780438  0.7700394595828238 12.2001609218852387   F   F   F
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0.6167580046523641	2.9205028833781403	13.7573467757868890	F	F	F
4.4598299963014023	1.0419000867645432	15.2066899140808065	T	T	T
0.5955766784875403	2.7624549114077528	16.4874975708078111	T	T	T
0.6595694401927786	6.6298917670073765	16.6306244656638142	T	T	T
4.3726357391256681	4.7108932949687157	15.0224619131353041	T	T	T
0.7058030603129238	6.4672753136124310	13.5580209908492506	F	F	F
4.4086996711235455	4.8191266125708356	12.3204488991888113	F	F	F
5.6715363344849337	6.6372158906857983	16.7295640226651869	T	T	T
5.6758822732918386	6.7313330050628108	13.5907646217275762	F	F	F
1.8905265783182470	0.9333255642403494	12.2256103096605884	F	F	F
1.8955280222627293	0.8095950366631618	15.1372923179934915	T	T	T
1.8911333370901573	4.7922906983272124	14.9933552225775539	T	T	T
1.8906033418294066	4.7507750788174317	12.3122395822918413	F	F	F
5.6760058693227018	2.7213904474369603	13.7206604568794788	F	F	F
5.6970983471609786	2.8479425945288628	16.5540943451909683	T	T	T
0.5684923931206077	4.6410324770634208	13.6140349333837065	F	F	F
4.3800115540927473	6.5296561451253972	12.2234202596149473	F	F	F
4.3442587060966975	2.9486435489481502	15.1959383163860799	T	T	T
0.5926018137849951	0.9524589336778226	16.4720396136118907	T	T	T
6.9939818398781295	2.9481451738415072	15.1665511006715370	T	T	T
3.1478763479569403	0.9913081112179767	16.5370661217147656	T	T	T
3.2123063240941336	4.6409616849872153	13.6140049494892601	F	F	F
6.9719322530726959	6.5297105535807285	12.2233730105456431	F	F	F
5.6757780022636899	0.9494924830044873	13.6748354828937444	F	F	F
5.6778678740859387	0.9797558477379603	16.6289486004559208	T	T	T
5.6856444982232688	5.7978056058247960	15.1620893114311581	T	T	T
1.8890395068721033	6.5631026136046655	15.1255451784395127	T	T	T
1.8904629143660816	6.6180150951668049	12.2590327337071869	F	F	F
1.8905788580977576	1.9229954669488631	13.6963480075419035	F	F	F
1.8626546536383513	3.9015925934685871	16.5217620367443843	T	T	T
5.6759058834275962	3.7912082295675131	12.2955930440659955	F	F	F
3.1440281353629915	6.8840654030338095	19.3477178435065227	T	T	T
6.9542162638692986	4.8414244473180794	18.2128095519197721	T	T	T
7.0051008218979200	0.9165916372512771	17.9400353144379778	T	T	T
2.5956216384049275	2.0863792781846495	19.6993687002750413	T	T	T
4.3795923489476554	0.8677695136849836	17.8145682298587005	T	T	T
0.0031350975207863	2.9690392245461226	19.5957807886107531	T	T	T
0.6541063419969099	6.4949488602451924	19.3836304585879660	T	T	T
4.4640896209425085	4.6298407088208720	18.3397820253213055	T	T	T
5.5785006731515310	6.9754858800397423	19.4401536923266178	T	T	T
1.8138147269156839	0.8773347775933465	17.7928305146606576	T	T	T
1.9783406405727384	4.6155168225592202	18.1264576682182899	T	T	T
4.9478937699652974	2.6220792561471082	19.6299485151719715	T	T	T
0.6941165533553443	4.6216814194769977	19.4219411966920212	T	T	T
4.3877519971558847	6.3782078487286666	18.0719937002459083	T	T	T
3.3072636989576698	3.6898202577053798	19.2635890206419198	T	T	T
6.8912960098922946	6.6182715968042141	18.1526533071992198	T	T	T
4.1314642957548626	0.9136680605247768	19.5881542120532686	T	T	T
1.9087698069439114	6.5813408130319662	18.0513130688209777	T	T	T
0.9009527014628995	1.4511333919812914	19.2637096480266443	T	T	T
5.8900027181211509	3.4837787314159820	18.3030888847495135	T	T	T
0.7695718132837671	0.8643452656042820	21.0302892050502201	T	T	T
4.1650581448398176	0.7294980803795666	21.4585957580800297	T	T	T
2.2684109977451463	4.5169958682510591	20.5572051276724217	T	T	T
0.0493213405334694	-0.8649217673222045	21.4845604223821915	T	T	T
2.3313910889911278	0.8186229132152404	23.8093913732227485	T	T	T
1.0886848521344465	-0.3951408970171723	25.5799170793549280	T	T	T
-0.1581608162254693	2.4706887884194271	21.6375894294955025	T	T	T
2.4035781866133661	3.3430691186117412	23.8853360064669147	T	T	T
1.1019908186408547	2.0801880895557101	25.5912092229658903	T	T	T
1.1447858041120558	4.5816961517784804	22.1850591243736446	T	T	T
2.3869083793655648	5.9337841873966646	23.8282958947362431	T	T	T
1.1107599440982516	4.6504448746085885	25.5992851519535733	T	T	T

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  2.5673823604366866 -0.6504992557554096 21.5452723894159313   T   T   T
  4.8746876938116124  0.8834187002276922 23.5689477933435789   T   T   T
  3.6544010656701729 -0.3853295102395843 25.5575752193821124   T   T   T
  2.3886108449580057  2.1502722622458670 21.7763336499059967   T   T   T
  4.9001488423098429  3.4032839824714545 23.8573688790473355   T   T   T
  3.6509895283346658  2.0783870551283217 25.5765612657655943   T   T   T
  3.6642487434273714  4.6583263920079778 22.0649425537682262   T   T   T
  4.9010324157173919  5.9530056597902039 23.7435363336599288   T   T   T
  3.6519865680356962  4.6634289682358778 25.6015047024192484   T   T   T
  5.1937252907368263 -1.0078068975411603 21.3508664729860307   T   T   T
  7.3868606118266786  0.8579615183146342 23.6452820353500179   T   T   T
  6.1413839150342158 -0.3754858009862180 25.5123418753627966   T   T   T
  4.9901970016720805  2.5873016223675758 21.6379793157797806   T   T   T
  7.4322913445801682  3.3502771255374060 23.8788814276961929   T   T   T
  6.1422829613789496  2.0818949926290897 25.5401867402451010   T   T   T
  6.2527808426365246  4.5993604054410309 22.0886326149039256   T   T   T
  7.4347864790058189  5.9422775125870446 23.7976491071224778   T   T   T
  6.1616409077038679  4.6699778733980422 25.6057020973774279   T   T   T
  2.3741903364213952  0.8475833645674378 27.3942505288986062   T   T   T
  1.1076684609562657 -0.4072246833623528 29.1613546632158638   T   T   T
  2.3761153756087974  3.3708576404069190 27.3618235233541505   T   T   T
  1.1081746728915687  2.1187570462519734 29.1475419438557743   T   T   T
  2.3739961116937600  5.9166760874852971 27.3718914338239010   T   T   T
  1.1102683776131077  4.6399220586322789 29.1250400079694387   T   T   T
  4.9029092040669582  0.8507340711768961 27.3894321635104703   T   T   T
  3.6321605331374918 -0.4071765228465685 29.1689409281252736   T   T   T
  4.9004549100211028  3.3710468284529811 27.3652684386894798   T   T   T
  3.6335814739658434  2.1212136867514322 29.1525181542630918   T   T   T
  4.9013870930605687  5.9244831055918290 27.3794892511060795   T   T   T
  3.6345038548526971  4.6428276431009641 29.1281762300227527   T   T   T
  7.4020439023864384  0.8507542035257473 27.3844870077737532   T   T   T
  6.1561772499584793 -0.4068820707280491 29.1719135053498526   T   T   T
  7.4142271235207060  3.3664728196920106 27.3621549524786118   T   T   T
  6.1562486955655213  2.1209816627533109 29.1586925561458159   T   T   T
  7.4127777993165767  5.9207780745330716 27.3776020792748263   T   T   T
  6.1590904893861023  4.6407093697468467 29.1338486408976749   T   T   T

Oxide reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Cu E_tot= -694.03663705 eV
 D3-zero damping= -12.7448531 eV, D3-BJ damping= -19.2314148 eV
 O Al  O Al  O Al  H  O  H  O  H  O  H
 1.0000000000000000
     7.5713089101900026    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.5713089101900026    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.2904852797336304
  18  12  24  16  12   8   1   1   1   1   1   1   3
Selective dynamics
Cartesian
  3.0742706814383642  6.7965354071552930 10.9423958550990683   F   F   F
  6.9496160755450562  4.6461529487152262  9.3854545373318246   F   F   F
  3.0752007950165097  6.4675089756823914  8.0000187449185951   F   F   F
  3.1643082791158981  2.9204295489932952  8.1990827428381010   F   F   F
  6.8608430427428830  1.0991113643589845  9.5845317789161761   F   F   F
  3.1579568896376000  2.7472501105824416 10.8220669229527680   F   F   F
  0.6167580046523641  2.9205028833781403  8.1993257849376420   F   F   F
  4.4914896717292514  1.0990167280483447  9.5846030099037201   F   F   F
  0.6234568781037551  2.7471348797031352 10.8217845066302907   F   F   F
  0.7068216598067383  6.7966335472545181 10.9423584978630899   F   F   F
  4.4019571249731957  4.6462339086007374  9.3853700880230981   F   F   F
  0.7058030603129238  6.4672753136124310  8.0000000000000000   F   F   F
  5.6759218341858286  6.6332349909229507 10.9172067463060039   F   F   F
  5.6758822732918386  6.7313330050628108  8.0327436308783255   F   F   F
  1.8908285973753074  0.8351705312417778  9.5519775531218265   F   F   F
  1.8907256769869536  4.8451065823013115  9.4220834377914784   F   F   F
```

5.6760058693227018	2.7213904474369603	8.1626394660302282	F	F	F
5.6760812370181952	2.8156935438133313	10.8301543211852653	F	F	F
0.5684923931206077	4.6410324770634208	8.0560139425344559	F	F	F
4.3541726304528670	2.9256773813273207	9.5285274732362595	F	F	F
0.5945048895347544	1.0367489316290468	10.9191009939757393	F	F	F
6.9979689459477150	2.9256281990931861	9.5284873332419124	F	F	F
3.1864724694090163	1.0368047279410977	10.9192047381793671	F	F	F
3.2123063240941336	4.6409616849872153	8.0559839586400095	F	F	F
5.6757780022636899	0.9494924830044873	8.1168144920444938	F	F	F
5.6761137094586616	0.9487371739588352	10.8835529458276739	F	F	F
5.6758398312500882	5.6436288270516490	9.4463612987341499	F	F	F
1.8908929283971920	6.6170420180407037	9.4677862360962415	F	F	F
1.8905788580977576	1.9229954669488631	8.1383270166926529	F	F	F
1.8906804002363682	3.7751923370469673	10.8469192662674665	F	F	F
3.1084435140042630	6.6942658078242188	16.7165047591137146	T	T	T
6.9944686816759001	4.6937286509388150	15.0223233430227250	T	T	T
3.0752007950165097	6.4675089756823914	13.5580397357678457	F	F	F
6.9431163702665497	4.8192064301244377	12.3205669558782276	F	F	F
6.8596658874772460	0.7701121542613976	12.2001224306209899	F	F	F
3.1643082791158981	2.9204295489932952	13.7571037336873516	F	F	F
6.9043491543253399	1.0114770476900998	15.1827416385449219	T	T	T
3.1721570904880170	2.7915931292105847	16.5257717252787657	T	T	T
4.4921781666780438	0.7700394595828238	12.2001609218852387	F	F	F
0.6167580046523641	2.9205028833781403	13.7573467757868890	F	F	F
4.4433098217850073	1.0092731545855209	15.2427511669328659	T	T	T
0.5862267334271584	2.7957919374792746	16.5224270706466498	T	T	T
0.7128604343957674	6.6861358314657942	16.6720865449770699	T	T	T
4.3630337248159474	4.7024794173323361	15.0269740465990882	T	T	T
0.7058030603129238	6.4672753136124310	13.5580209908492506	F	F	F
4.4086996711235455	4.8191266125708356	12.3204488991888113	F	F	F
5.6924260293791473	6.5938329086311382	16.6748998716882468	T	T	T
5.6758822732918386	6.7313330050628108	13.5907646217275762	F	F	F
1.8905265783182470	0.9333255642403494	12.2256103096605884	F	F	F
1.8956136799938166	0.8447052321481533	15.2131548707146838	T	T	T
1.8955421958704017	4.8168575525361277	15.0403697053310239	T	T	T
1.8906033418294066	4.7507750788174317	12.3122395822918413	F	F	F
5.6760058693227018	2.7213904474369603	13.7206604568794788	F	F	F
5.6756689290726934	2.8124088663622291	16.4377461470653508	T	T	T
0.5684923931206077	4.6410324770634208	13.6140349333837065	F	F	F
4.3800115540927473	6.5296561451253972	12.2234202596149473	F	F	F
4.3262806277421744	2.9272694523858567	15.1587155767117103	T	T	T
0.5995784553790162	1.0173215881982141	16.6014007945937578	T	T	T
7.0168976295834362	2.9178833465773533	15.1377619027744998	T	T	T
3.1571221806130949	1.0268082834904848	16.6252748336621927	T	T	T
3.2123063240941336	4.6409616849872153	13.6140049494892601	F	F	F
6.9719322530726959	6.5297105535807285	12.2233730105456431	F	F	F
5.6757780022636899	0.9494924830044873	13.6748354828937444	F	F	F
5.6928062056773427	0.9307389117362554	16.5943938394985153	T	T	T
5.6854478253703995	5.7741536645652634	15.1052952950685064	T	T	T
1.8776555592746391	6.5994143371467739	15.1221771075498701	T	T	T
1.8904629143660816	6.6180150951668049	12.2590327337071869	F	F	F
1.8905788580977576	1.9229954669488631	13.6963480075419035	F	F	F
1.8757336744599757	3.9194612276057135	16.5835119748811337	T	T	T
5.6759058834275962	3.7912082295675131	12.2955930440659955	F	F	F
3.2254172140328254	6.3807120925758802	19.3693909813431979	T	T	T
7.0495861506536759	4.7539580154491334	18.1665247014740032	T	T	T
6.9304354008067746	0.8591455313556301	17.8740587046729473	T	T	T
3.1089441065232353	2.6465015243621108	19.7412111865697533	T	T	T
4.4135748930571488	0.8313311163182893	17.9626582212871746	T	T	T
0.4192181644490312	2.9907129812222459	20.0336096542620936	T	T	T
0.6484760046189848	6.5119069343482732	19.4149191964473360	T	T	T
4.4089493660836263	4.6129722607916950	18.1490625829839693	T	T	T
5.6826581141675474	6.5230499318379920	19.3354460572600040	T	T	T

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  1.8705544643090206  0.9494484499003044 18.0468404463656995   T   T   T
  1.9288208694709648  4.6740215730960344 18.1906386255923422   T   T   T
  5.7282683236679217  2.7587685378522688 19.5383661391413064   T   T   T
  0.6335408023348826  4.6998901873489336 19.5283402412455516   T   T   T
  4.4438604532283223  6.4027885093766219 17.9720425045707408   T   T   T
  3.2326583403205200  4.4053137590138549 19.4383289654110740   T   T   T
  6.9837170484428315  6.5911177911059822 18.0802603774460628   T   T   T
  4.5026678181937143  1.5758555836733690 19.6079596873458257   T   T   T
  1.8879978603253580  6.6344852367136955 18.1173877065956859   T   T   T
  1.5728561033702426  1.7135855900649293 19.6979588438465321   T   T   T
  5.8077062388127514  3.6156095818709479 17.9904743083421081   T   T   T
  6.8856490606623062  2.7362515539104617 19.8920578319643973   T   T   T
  1.7206854049536633  0.7152181844864174 21.1223544151816647   T   T   T
  1.2960948265977059 -0.1567479447043622 21.0026362958283492   T   T   T
  4.3870157551795117  0.4737863385576153 20.9773606465900855   T   T   T
  3.5435884435154752  0.6267541650940259 21.4802669060663689   T   T   T
  2.0751943954040746  4.7691672160292882 20.8578032493441832   T   T   T
  1.9669145913361030  4.0133138402031285 21.4619250077356973   T   T   T
  3.5242970788369830  6.9678401253514179 20.1420044822846194   T   T   T
  5.5789813614318549  7.0043140063765019 20.1772679246644273   T   T   T

Metal reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Cu E_tot= -173.98184631 eV
 D3-zero damping= -16.8611412 eV, D3-BJ damping= -20.3780334 eV
Cu
 1.0000000000000000
     7.5713089101900026    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.5713089101900026    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0001559791606477 -0.0001563790284090  8.2531365685509641
  1.2619378323209398  1.2619375981006291 10.0242949591771566
 -0.0004063062167627 -0.0004063704229356 11.8276157489577916
  1.2616054292823389  1.2616055741405616 13.6312266804165656
 -0.0007399052426475 -0.0007396623845194 15.4025494126481295
 -0.0001686103269882  2.5232484381304197  8.2527595471933761
  1.2618696147409953  3.7853694565799700 10.0239414806670837
 -0.0004602357656926  2.5228570519187379 11.8275487974655409
  1.2615050351894372  3.7849893617214798 13.6314906343159770
 -0.0008100095988099  2.5227253726391883 15.4029435579470899
 -0.0001614081217112  5.0477400200425118  8.2527662706308327
  1.2619262122153880  6.3088348085377479 10.0242902633812516
 -0.0004621917150900  5.0475849334381016 11.8275558915558250
  1.2615874056631262  6.3084712697320766 13.6311672322289734
 -0.0008020332643568  5.0471719978963048 15.4028927199030310
  2.5232487966725694 -0.0001690284560401  8.2527595471933761
  3.7853696606272274  1.2618691962840287 10.0239414029962095
  2.5228571045061132 -0.0004601549088411 11.8275488157268303
  3.7849891660070987  1.2615052529052411 13.6314905621286435
  2.5227251819351508 -0.0008096954184889 15.4029435579470899
  2.5230533828103936  2.5230530719321145  8.2523450237744935
  3.7853780238854244  3.7853775516870192 10.0233021369657642
  2.5229972569386740  2.5229973267832593 11.8274970264182269
  3.7849736189709509  3.7849739019951194 13.6320275080877398
  2.5225065726209701  2.5225068267851767 15.4033327417629913
  2.5230529200473897  5.0479261121161345  8.2523530227240940
  3.7853713796963366  6.3088788069057697 10.0239140941770923
  2.5229740513414893  5.0474803400900452 11.8274927687177804
  3.7849929777958331  6.3084802598539955 13.6314159874857186
  2.5225038986044921  5.0473588501023503 15.4032685334809081
  5.0477403110716459 -0.0001619528299373  8.2527664067188251
  6.3088350069159995  1.2619258332322529 10.0242902172011945
  5.0475849023970722 -0.0004621753603053 11.8275558858868255
```

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  6.3084709974401738  1.2615876285602672 13.6311671543283257
  5.0471717693820271 -0.0008016461524593 15.4028927055591875
  5.0479263553092810  2.5230525043766474  8.2523529959808233
  6.3088790654110456  3.7853709335689403 10.0239139942556026
  5.0474803035183022  2.5229740101384666 11.8274927687177804
  6.3084800641396130  3.7849932062237115 13.6314159247075253
  5.0473586302403328  2.5225042103183655 15.4032683622334012
  5.0479345074322346  5.0479341625935881  8.2523438779395590
  6.3088448741306662  6.3088445895543890 10.0242871343149389
  5.0474931046530571  5.0474932524176923 11.8274913241470347
  6.3084910976839188  6.3084913059905903 13.6311069154961402
  5.0473671385732413  5.0473673794631546 15.4032329402729857

Interface: 3O-g-Al2O3(110)/fcc(100)_3x3/Pt E_tot= -971.1506563 eV
 D3-zero damping= -40.8836241 eV, D3-BJ damping= -46.5138123 eV
 O Al  O Al  O Al  O Pt
 1.0000000000000000
     8.3113600962600014    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.3113600962600014    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.3375309279805094
  18  12  24  16  12   8   3  45
Selective dynamics
Cartesian
  3.3747626691627945  7.4608570124278737 10.9423958550990701   F   F   F
  7.6289004212829958  5.1002872392513972  9.3854545373318263   F   F   F
  3.3757836959060024  7.0996701706813692  8.0000187449185969   F   F   F
  3.4736009156769483  3.2058844653364353  8.1990827428381028   F   F   F
  7.5314503434684532  1.2065430751061383  9.5845317789161779   F   F   F
  3.4666287150057160  3.0157777491828393 10.8220669229527697   F   F   F
  0.6770424942003799  3.2059649677287059  8.1993257849376437   F   F   F
  4.9305065310613019  1.2064391886493528  9.5846030099037218   F   F   F
  0.6843961433717738  3.0156512551586903 10.8217845066302925   F   F   F
  0.7759093451574097  7.4609647451480958 10.9423584978630917   F   F   F
  4.8322227012438042  5.1003761124924463  9.3853700880230999   F   F   F
  0.7747911835175424  7.0994136695099979  8.0000000000000018   F   F   F
  6.2307100135158962  7.2815949351205465 10.9172067463060056   F   F   F
  6.2306665857757810  7.3892814566871223  8.0327436308783273   F   F   F
  2.0756460394769469  0.9168035684811312  9.5519775531218283   F   F   F
  2.0755330592222774  5.3186874274893681  9.4220834377914802   F   F   F
  6.2308022625961508  2.9873904551337462  8.1626394660302299   F   F   F
  6.2308849970432991  3.0909111279095538 10.8301543211852671   F   F   F
  0.6240592012895958  5.0946662714285722  8.0560139425344577   F   F   F
  4.7797675517198304  3.2116452426036499  9.5285274732362613   F   F   F
  0.6526142671659424  1.1380850791313979 10.9191009939757411   F   F   F
  7.6819795021092201  3.2115912530936352  9.5284873332419142   F   F   F
  3.4979315260051318  1.1381463292067810 10.9192047381793689   F   F   F
  3.5262904889677289  5.0945885598407497  8.0559839586400113   F   F   F
  6.2305521228641716  1.0422998227322735  8.1168144920444956   F   F   F
  6.2309206434749953  1.0414706866427490 10.8835529458276756   F   F   F
  6.2306199952725541  6.1952605537108631  9.4463612987341516   F   F   F
  2.0757166584801583  7.2638191937989633  9.4677862360962433   F   F   F
  2.0753718896449276  2.1109570325121711  8.1383270166926547   F   F   F
  2.0754833569339985  4.1441953192015903 10.8469192662674683   F   F   F
  3.3833985184659148  7.4790989474068041 16.4383134832099493   T   T   T
  7.6207260623739996  5.0600978433836445 14.9407886294978773   T   T   T
  3.3757836959060024  7.0996701706813692 13.5580397357678475   F   F   F
  7.6217654078091011  5.2902556868427526 12.3205669558782294   F   F   F
  7.5301581281569430  0.8453861154652559 12.2001224306209917   F   F   F
  3.4736009156769483  3.2058844653364353 13.7571037336873534   F   F   F
  7.5144292418549155  1.2350663895735394 15.0717803835727189   T   T   T
  3.4458593290535791  2.9441537140100453 16.3024919684605649   T   T   T
  4.9312623223665764  0.8453063153068058 12.2001609218852405   F   F   F
  0.6770424942003799  3.2059649677287059 13.7573467757868908   F   F   F
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4.9607106897278275	1.2169715699093631	15.1296102906319057	T	T	T
0.6893433595902659	2.9450247025388610	16.3577096151296146	T	T	T
0.8295683928526311	7.4186953235134103	16.4142910379044942	T	T	T
4.8410536638804222	5.0618563612935858	14.9334432615338386	T	T	T
0.7747911835175424	7.0994136695099979	13.5580209908492524	F	F	F
4.8396242918651815	5.2901680675898790	12.3204488991888130	F	F	F
6.2064725300664527	7.2496382684637943	16.4443216125981415	T	T	T
6.2306665857757810	7.3892814566871223	13.5907646217275779	F	F	F
2.0753144998225834	1.0245526821665401	12.2256103096605901	F	F	F
2.0730906750640004	0.8948000997637237	15.0441846867593778	T	T	T
2.0820454278988461	5.2955627610657219	14.9247167388519113	T	T	T
2.0753987665182199	5.2151355709773535	12.3122395822918431	F	F	F
6.2308022625961508	2.9873904551337462	13.7206604568794805	F	F	F
6.2326274566725761	3.0693866898477644	16.4160747690543296	T	T	T
0.6240592012895958	5.0946662714285722	13.6140349333837083	F	F	F
4.8081320790978870	7.1678918626412527	12.2234202596149490	F	F	F
4.8008322383460138	3.2027353809275048	15.0775982146354188	T	T	T
0.6276931122843499	1.0667830697443650	16.3763491634636935	T	T	T
7.6702278291297619	3.1935828804362947	15.0826193500413392	T	T	T
3.4881681609089141	1.0890035205713011	16.3431643844434404	T	T	T
3.5262904889677289	5.0945885598407497	13.6140049494892619	F	F	F
7.6533978747093974	7.1679515892050354	12.2233730105456448	F	F	F
6.2305521228641716	1.0422998227322735	13.6748354828937462	F	F	F
6.2615091815198740	1.0823434389545721	16.5109372297606321	T	T	T
6.2287146846101731	6.1715829850297341	14.9992884140378333	T	T	T
2.0840902605366001	7.2240306615859549	15.0438933522331766	T	T	T
2.0752446130912570	7.2648873835257861	12.2590327337071887	F	F	F
2.0753718896449276	2.1109570325121711	13.6963480075419053	F	F	F
2.0651750660853581	4.0572798733536928	16.2709407938502046	T	T	T
6.2306925036642893	4.1617766715912810	12.2955930440659973	F	F	F
3.4767917243343560	6.9280705453907094	18.9388768638650049	T	T	T
7.6179855111699446	5.1997775211369213	17.9208073487679052	T	T	T
7.6349529502822797	0.7713218115657948	17.6021536395961071	T	T	T
3.4787221855953989	3.2160094193103519	19.0146586246462483	T	T	T
4.8148611295952595	0.8917768292667154	17.7090561454316386	T	T	T
0.6552756349837990	3.2142014846172846	19.4831654782089920	T	T	T
0.7184232813908307	6.9827474812026207	18.9454440458805031	T	T	T
4.9021396067283511	5.2186112253977308	17.8639399152889702	T	T	T
6.2661081895417485	7.2435944055848163	18.9666702310403110	T	T	T
2.0497509717499169	1.0047021550456323	17.7220045478003847	T	T	T
2.0507063686466531	5.0697640264715673	17.7243159429937727	T	T	T
6.0803496318600505	3.0095463758311958	19.3090997968226752	T	T	T
0.7038636592684252	5.0853733551390068	18.9822319100341801	T	T	T
4.8509323570870038	7.0955339578098187	17.7625431497730801	T	T	T
3.4591266773548943	5.0444221744895570	18.8881890303159459	T	T	T
7.6625279378625679	7.1893566542390257	17.7411647234130996	T	T	T
4.7428304498902101	1.8146326808291164	19.2647017310730853	T	T	T
2.0923675039025782	7.3799677411483406	17.8695976082583172	T	T	T
2.0186143363119027	2.1700929641423787	19.0845794121279191	T	T	T
6.2659686122857430	4.1109256734483957	17.9150402499706445	T	T	T
3.1443482446846889	1.2036824957244197	20.1744733360933388	T	T	T
5.6415909869692529	0.8525029632723724	20.6607331560862626	T	T	T
2.0407732787210411	5.1956664551081113	20.3347918880490219	T	T	T
0.6996067295205889	0.0508622983091311	21.7292414643603031	T	T	T
1.8831983607448863	1.4294109392283070	23.6924654164903608	T	T	T
0.4670230134898289	0.0404512253776574	25.5740421988005124	T	T	T
0.5048297256409452	2.7399437647149938	21.5318150911782027	T	T	T
1.8493646594207906	4.1840978958976534	23.6677218102619165	T	T	T
0.4959375251163272	2.7957371156320430	25.6450568851466514	T	T	T
0.3976959898603430	5.6314196877672043	21.6697477067372226	T	T	T
1.9087803293709147	6.9386286592358788	23.7137866943781965	T	T	T
0.4792066117807620	5.5857956284375891	25.6051288751911201	T	T	T
3.3552340467188473	-0.1322359449164232	21.6960635572183840	T	T	T

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  4.7136510249868655  1.3450354454603806 23.6509334622006442   T   T   T
  3.2809056843957034  0.0230519717283170 25.6303598078457320   T   T   T
  3.3219435784514100  2.7714874669621521 21.8086865652775757   T   T   T
  4.6534231447787961  4.1020406765342194 23.7163860896276546   T   T   T
  3.2563553048174172  2.7815373740854428 25.6481548340059433   T   T   T
  3.4273346336980453  5.5046514922614698 21.7465530251840775   T   T   T
  4.6694433814067517  6.9361424210170988 23.6123797712430097   T   T   T
  3.2578659203282010  5.5494832384928268 25.6425147897181454   T   T   T
  6.7759495610100871 -0.7846426876817330 20.8336176988429536   T   T   T
  7.4092359805843424  1.4345392273774749 23.5195283599315452   T   T   T
  6.0605472946007444 -0.0001901579398360 25.5642849459571018   T   T   T
  6.1274469726835488  2.6991444778743081 21.4394306380642874   T   T   T
  7.4526824481077680  4.1190090532535342 23.6941036810070180   T   T   T
  6.0432619346491467  2.7527789933398790 25.6158908397946057   T   T   T
  6.0367474075408962  5.2763422578010166 21.7509929697697544   T   T   T
  7.3628349415605783  6.9896170227177050 23.5211166823956184   T   T   T
  6.0308997347419213  5.5603575369048892 25.5808211152045430   T   T   T
  1.8780553691565158  1.3976172097985029 27.5831057102573496   T   T   T
  0.4941058549141618  0.0157507400978683 29.5201272333615670   T   T   T
  1.8811456177146717  4.1762957880929994 27.6008660356787026   T   T   T
  0.5005678349507439  2.7876870813558141 29.5211272073360647   T   T   T
  1.8779231700759238  6.9500352655083191 27.5670974908952786   T   T   T
  0.4908394873030235  5.5713923011788982 29.5118421397093549   T   T   T
  4.6583576234647888  1.3905443021975004 27.5709591340195708   T   T   T
  3.2749597292149115  0.0091195908777909 29.5124092615727385   T   T   T
  4.6576932752486648  4.1646240114746291 27.5730720674919496   T   T   T
  3.2727237984459276  2.7780363838903321 29.5403638016658654   T   T   T
  4.6563571882837742  6.9345424311543491 27.5597679885816653   T   T   T
  3.2747215655812694  5.5515699414639030 29.5155912606135864   T   T   T
  7.4266821292830718  1.3943988774259450 27.5650998138904626   T   T   T
  6.0466943848849164 -0.0015011464706261 29.4989525346880654   T   T   T
  7.4228562347816540  4.1744912751207472 27.5602059400079185   T   T   T
  6.0370830468792915  2.7785647153682240 29.5068106777976240   T   T   T
  7.4238784623914027  6.9457595016717653 27.5384670640727762   T   T   T
  6.0429309827777953  5.5552667117749017 29.5016419836445465   T   T   T

Oxide reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Pt E_tot= -710.46561545 eV
 D3-zero damping= -10.9103846 eV, D3-BJ damping= -16.3470596 eV
 O Al  O Al  O Al  H  O  H  O  H  O  H
 1.0000000000000000
     8.3113600962600014    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.3113600962600014    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.2904852797336304
  18  12  24  16  12   8   1   1   1   1   1   1   3
Selective dynamics
Cartesian
  3.3747626691627945  7.4608570124278737 10.9423958550990683   F   F   F
  7.6289004212829958  5.1002872392513972  9.3854545373318246   F   F   F
  3.3757836959060024  7.0996701706813692  8.0000187449185951   F   F   F
  3.4736009156769483  3.2058844653364353  8.1990827428381010   F   F   F
  7.5314503434684532  1.2065430751061383  9.5845317789161761   F   F   F
  3.4666287150057160  3.0157777491828393 10.8220669229527680   F   F   F
  0.6770424942003799  3.2059649677287059  8.1993257849376420   F   F   F
  4.9305065310613019  1.2064391886493528  9.5846030099037201   F   F   F
  0.6843961433717738  3.0156512551586903 10.8217845066302907   F   F   F
  0.7759093451574097  7.4609647451480958 10.9423584978630899   F   F   F
  4.8322227012438042  5.1003761124924463  9.3853700880230981   F   F   F
  0.7747911835175424  7.0994136695099979  8.0000000000000000   F   F   F
  6.2307100135158962  7.2815949351205465 10.9172067463060039   F   F   F
  6.2306665857757810  7.3892814566871223  8.0327436308783255   F   F   F
  2.0756460394769469  0.9168035684811312  9.5519775531218265   F   F   F
  2.0755330592222774  5.3186874274893681  9.4220834377914784   F   F   F
  6.2308022625961508  2.9873904551337462  8.1626394660302282   F   F   F
```

6.2308849970432991	3.0909111279095538	10.8301543211852653	F	F	F
0.6240592012895958	5.0946662714285722	8.0560139425344559	F	F	F
4.7797675517198304	3.2116452426036499	9.5285274732362595	F	F	F
0.6526142671659424	1.1380850791313979	10.9191009939757393	F	F	F
7.6819795021092201	3.2115912530936352	9.5284873332419124	F	F	F
3.4979315260051318	1.1381463292067810	10.9192047381793671	F	F	F
3.5262904889677289	5.0945885598407497	8.0559839586400095	F	F	F
6.2305521228641716	1.0422998227322735	8.1168144920444938	F	F	F
6.2309206434749953	1.0414706866427490	10.8835529458276739	F	F	F
6.2306199952725541	6.1952605537108631	9.4463612987341499	F	F	F
2.0757166584801583	7.2638191937989633	9.4677862360962415	F	F	F
2.0753718896449276	2.1109570325121711	8.1383270166926529	F	F	F
2.0754833569339985	4.1441953192015903	10.8469192662674665	F	F	F
3.3686775450437025	7.4539359688930773	16.5050113134013969	T	T	T
7.6270693837932617	5.0641245860070496	14.9455814493298647	T	T	T
3.3757836959060024	7.0996701706813692	13.5580397357678457	F	F	F
7.6217654078091011	5.2902556868427526	12.3205669558782276	F	F	F
7.5301581281569430	0.8453861154652559	12.2001224306209899	F	F	F
3.4736009156769483	3.2058844653364353	13.7571037336873516	F	F	F
7.5069681778649695	1.2287721654230477	15.0859847223228538	T	T	T
3.4569802455163248	2.9751732913559823	16.3553723971344702	T	T	T
4.9312623223665764	0.8453063153068058	12.2001609218852387	F	F	F
0.6770424942003799	3.2059649677287059	13.7573467757868890	F	F	F
4.9453153570952368	1.2212761396711802	15.1440150723316513	T	T	T
0.6766482873602939	2.9492986167774862	16.3504722219867169	T	T	T
0.8172575781572141	7.4263091136348693	16.4274433009354937	T	T	T
4.8364235926358257	5.0688674520848220	14.9515471844008978	T	T	T
0.7747911835175424	7.0994136695099979	13.5580209908492506	F	F	F
4.8396242918651815	5.2901680675898790	12.3204488991888113	F	F	F
6.1886888410380960	7.2099931671617288	16.4556251864576737	T	T	T
6.2306665857757810	7.3892814566871223	13.5907646217275762	F	F	F
2.0753144998225834	1.0245526821665401	12.2256103096605884	F	F	F
2.0848250946927518	0.8994752515727352	15.0710708125658890	T	T	T
2.0798460104700873	5.3006242128276089	14.9416721883183961	T	T	T
2.0753987665182199	5.2151355709773535	12.3122395822918413	F	F	F
6.2308022625961508	2.9873904551337462	13.7206604568794788	F	F	F
6.2312447671429734	3.1015407998542099	16.3675488690253417	T	T	T
0.6240592012895958	5.0946662714285722	13.6140349333837065	F	F	F
4.8081320790978870	7.1678918626412527	12.2234202596149473	F	F	F
4.7935722785216903	3.2041623411854960	15.0671468920573073	T	T	T
0.6194550037597214	1.0735589218260506	16.3754300401395092	T	T	T
7.6658117752886890	3.1982509991762038	15.0594481070777526	T	T	T
3.4811480011231613	1.1168148616164417	16.3898871862851578	T	T	T
3.5262904889677289	5.0945885598407497	13.6140049494892601	F	F	F
7.6533978747093974	7.1679515892050354	12.2233730105456431	F	F	F
6.2305521228641716	1.0422998227322735	13.6748354828937444	F	F	F
6.2500287877928669	1.1085443889063022	16.5086770559839309	T	T	T
6.2361030973878666	6.1729947672867000	14.9783439669799705	T	T	T
2.0754747165428471	7.2262530200257586	15.0358366165546666	T	T	T
2.0752446130912570	7.2648873835257861	12.2590327337071869	F	F	F
2.0753718896449276	2.1109570325121711	13.6963480075419035	F	F	F
2.0512682364234931	4.0581318834877012	16.2729990012282251	T	T	T
6.2306925036642893	4.1617766715912810	12.2955930440659955	F	F	F
3.4507013601907608	7.0465239065505152	19.0020691611141821	T	T	T
7.5965227478019575	5.2681816870108342	17.9332639060379790	T	T	T
7.6204490728054592	0.7742462776619191	17.6176459852186653	T	T	T
3.3841523950187371	2.9497764835231615	19.3148232198325402	T	T	T
4.8269033472109975	0.9240235661004090	17.7094462793336049	T	T	T
0.5333046234050920	3.2982921323454275	19.4045447739982144	T	T	T
0.7078087941095801	6.9823192346379779	19.0064608609565155	T	T	T
4.8079981261705589	5.1758104648243037	17.9782033016983256	T	T	T
6.1748776289186678	7.2181216458219994	19.0004289515030074	T	T	T
2.0374120144883379	1.0152300002577648	17.7532688672393562	T	T	T

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  2.0865259612382956  5.0568147573017415 17.7596400191772439   T   T   T
  6.2143714800562657  3.0314071482878937 19.1928679311200057   T   T   T
  0.7227056412592143  5.1331675948261495 18.9869968719120301   T   T   T
  4.8338898098790359  7.0570839003629349 17.7234318880062069   T   T   T
  3.4038750976961079  4.7507889243452732 18.9563648421853941   T   T   T
  7.6081620817246627  7.2084112173979298 17.8142839968466404   T   T   T
  4.8901922938839135  1.9175713997748054 19.2433413237143753   T   T   T
  2.0283874053783273  7.4176450139275127 17.8581446642172921   T   T   T
  1.8147372056169866  2.0110945796537547 19.2715646772281666   T   T   T
  6.2585647314709156  4.1484409698633549 17.8482921354752087   T   T   T
  7.8708694093755742  2.9888223236562594 19.3917399745457111   T   T   T
  1.7258938981704857  0.9159575887405360 20.6010872178328022   T   T   T
  1.2340347044455484  0.0861239835257369 20.4381517673478221   T   T   T
  4.7831974599912517  0.6887638831677991 20.4968792074585160   T   T   T
  4.2836426775285306  0.8753603326207087 21.3073118618688788   T   T   T
  2.1889017244682778  5.1273624456458569 20.3123612355296750   T   T   T
  2.1107249078400772  4.4505646992460957 21.0052998122497847   T   T   T
  3.6340198451574808  7.6311491146268269 19.7836359628009326   T   T   T
  6.0282313576719204  7.8235440779062992 19.7549522811966334   T   T   T

Metal reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Pt E_tot= -284.83068848 eV
 D3-zero damping= -26.2261496 eV, D3-BJ damping= -26.788886 eV
Pt
 1.0000000000000000
     8.3113600962600014    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.3113600962600014    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0002044765405899 -0.0002052706292012  7.9297751302158259
  1.3851874200727903  1.3851868271119350  9.8759158461155288
 -0.0000789564021926 -0.0000790434411963 11.8275971545169813
  1.3844598001513646  1.3844602327809783 13.7795168648150987
 -0.0013794526760332 -0.0013785925153213 15.7257940782513437
 -0.0002044704573649  2.7702481277041540  7.9297750776975731
  1.3851874584032424  4.1556402746949885  9.8759158674847267
 -0.0000790126971761  2.7703744108857884 11.8275971785238116
  1.3844597903451614  4.1549135930138101 13.7795169273632698
 -0.0013794570870213  2.7690747606121153 15.7257941575337181
 -0.0002044765405899  5.5407014816328939  7.9297750743555797
  1.3851874055358107  6.9260935368843857  9.8759158376617666
 -0.0000789763343884  5.5408277514083295 11.8275971544105563
  1.3844597618209131  6.9253669194255805 13.7795168650259701
 -0.0013794740671052  5.5395281433485488 15.7257940853902323
  2.7702489115747184 -0.0002051606745426  7.9297750902131376
  4.1556407447508850  1.3851868315229232  9.8759158630020085
  2.7703744006519400 -0.0000790194124838 11.8275971221442848
  4.1549131329634328  1.3844601988615139 13.7795168841839679
  2.7690738543233322 -0.0013785925153213 15.7257940796883435
  2.7702489698373651  2.7702481776228187  7.9297750139014145
  4.1556408194122572  4.1556402471328013  9.8759158477658975
  2.7703744338005380  2.7703744254227680 11.8275971446043524
  4.1549131415426563  4.1549135728388595 13.7795169065404366
  2.7690739509164306  2.7690747606121153 15.7257942332325609
  2.7702489499051697  5.5407015155523558  7.9297749760902381
  4.1556406933952275  6.9260935179364163  9.8759157827857589
  2.7703744410788711  5.5408277692473860 11.8275971819727417
  4.1549131317364507  6.9253669286820729 13.7795169351901592
  2.7690738866960296  5.5395281433485488 15.7257940741733684
  5.5407022698743731 -0.0002051864766026  7.9297751177753248
  6.9260941207257849  1.3851868478997640  9.8759158685969712
  5.5408277446989009 -0.0000790646499239 11.8275971185889333
  6.9253664723737192  1.3844602042567304 13.7795168886085708
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  5.5395272876338169 -0.0013786284433729 15.7257941106240420
  5.5407022698743731  2.7702481117301794  7.9297750702809413
  6.9260941277932453  4.1556402427218107  9.8759158606306325
  5.5408277762990412  2.7703743978605804 11.8275971683978245
  6.9253664637944947  4.1549136111693121 13.7795168904916849
  5.5395272876338169  2.7690747496304882 15.7257940967432113
  5.5407022458456616  5.5407014233702458  7.9297750419828823
  6.9260940823953332  6.9260935223474061  9.8759157783611560
  5.5408277465606437  5.5408276968686625 11.8275971819727417
  6.9253664848175527  6.9253669108463551 13.7795168791387148
  5.5395272876338169  5.5395280755941663 15.7257941164620458

Interface: 3O-g-Al2O3(110)/fcc(100)_3x3/Pd E_tot= -927.58605227 eV
 D3-zero damping= -34.2853361 eV, D3-BJ damping= -42.8687506 eV
 O Al  O Al  O Al  O Pd
 1.0000000000000000
     8.2439436957000023    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.2439436957000023    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.3375309279805094
  18  12  24  16  12   8   3  45
Selective dynamics
Cartesian
  3.3473887677478400  7.4003393451573807 10.9423958550990701   F   F   F
  7.5670196941003303  5.0589169937668892  9.3854545373318263   F   F   F
  3.3484015125796511  7.0420822184657137  8.0000187449185969   F   F   F
  3.4454253020583985  3.1798803951528498  8.1990827428381028   F   F   F
  7.4703600685588762  1.1967563746982413  9.5845317789161779   F   F   F
  3.4385096553888932  2.9913157022513954 10.8220669229527697   F   F   F
  0.6715507615048258  3.1799602445615576  8.1993257849376437   F   F   F
  4.8905134373423458  1.1966533309014900  9.5846030099037218   F   F   F
  0.6788447626099137  2.9911902342653081 10.8217845066302925   F   F   F
  0.7696156682374413  7.4004462040191576 10.9423584978630917   F   F   F
  4.7930268226572466  5.0590051461254415  9.3853700880230999   F   F   F
  0.7685065764046971  7.0418277978666568  8.0000000000000018   F   F   F
  6.1801705064822157  7.2225313263758544 10.9172067463060056   F   F   F
  6.1801274309999608  7.3293443642299252  8.0327436308783273   F   F   F
  2.0588097355269928  0.9093670483578636  9.5519775531218283   F   F   F
  2.0586976716953895  5.2755456603282509  9.4220834377914802   F   F   F
  6.1802620072973404  2.9631586676501263  8.1626394660302299   F   F   F
  6.1803440706559343  3.0658396473960003 10.8301543211852671   F   F   F
  0.6189972349447344  5.0533416196151224  8.0560139425344577   F   F   F
  4.7409971555249371  3.1855944447048308  9.5285274732362613   F   F   F
  0.6473206805162403  1.1288536658996928 10.9191009939757411   F   F   F
  7.6196682316059796  3.1855408931229516  9.5284873332419142   F   F   F
  3.4695585581445858  1.1289144191539098 10.9192047381793689   F   F   F
  3.4976874914628877  5.0532645383736545  8.0559839586400113   F   F   F
  6.1800138965377762  1.0338453578144855  8.1168144920444956   F   F   F
  6.1803794279467335  1.0330229471429531 10.8835529458276756   F   F   F
  6.1800812184088922  6.1450085898655633  9.4463612987341516   F   F   F
  2.0588797817143289  7.2048997704202415  9.4677862360962433   F   F   F
  2.0585378094218574  2.0938343085271010  8.1383270166926547   F   F   F
  2.0586483725600648  4.1105802756464582 10.8469192662674683   F   F   F
  3.3575560068468109  7.4144793160269877 16.4567814296796335   T   T   T
  7.5616271230750867  5.0284628608187507 14.9468894338220686   T   T   T
  3.3484015125796511  7.0420822184657137 13.5580397357678475   F   F   F
  7.5599425552607658  5.2473445396516336 12.3205669558782294   F   F   F
  7.4690783348657828  0.8385288877277990 12.2001224306209917   F   F   F
  3.4454253020583985  3.1798803951528498 13.7571037336873534   F   F   F
  7.4585236761566609  1.2173932564727667 15.0849396701637577   T   T   T
  3.4124932444869893  2.9308618824912549 16.3076718813885897   T   T   T
  4.8912630981552843  0.8384497348568426 12.2001609218852405   F   F   F
  0.6715507615048258  3.1799602445615576 13.7573467757868908   F   F   F
  4.9134350543122656  1.2028750798760177 15.1401663141081535   T   T   T
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0.6841710489873132	2.9355972140767115	16.3726891246926307	T	T	T
0.8113423035492818	7.3462876442715057	16.4527981142048318	T	T	T
4.7974958125372238	5.0288660518186497	14.9388301280188056	T	T	T
0.7685065764046971	7.0418277978666568	13.5580209908492524	F	F	F
4.8003683763421492	5.2472576311097123	12.3204488991888130	F	F	F
6.1594429849945138	7.2164527967846057	16.4562081381269500	T	T	T
6.1801274309999608	7.3293443642299252	13.5907646217275779	F	F	F
2.0584808851087932	1.0162421706238094	12.2256103096605901	F	F	F
2.0486270240989470	0.8829293410620966	15.0507774051711536	T	T	T
2.0631889100789294	5.2585747396620794	14.9251112860190300	T	T	T
2.0585644682872624	5.1728337497885555	12.3122395822918431	F	F	F
6.1802620072973404	2.9631586676501263	13.7206604568794805	F	F	F
6.1838159048440495	3.0495929546186917	16.4176038240075215	T	T	T
0.6189972349447344	5.0533416196151224	13.6140349333837083	F	F	F
4.7691316081237431	7.1097505399953924	12.2234202596149490	F	F	F
4.7600787229027652	3.1786892779736409	15.0854699789163451	T	T	T
0.6201128679184561	1.0585567519107895	16.3939105062421220	T	T	T
7.6090114216336211	3.1709814924417530	15.0907834443071209	T	T	T
3.4545447074875550	1.0810465589561360	16.3596033316601464	T	T	T
3.4976874914628877	5.0532645383736545	13.6140049494892619	F	F	F
7.5913184399609710	7.1098097820957546	12.2233730105456448	F	F	F
6.1800138965377762	1.0338453578144855	13.6748354828937462	F	F	F
6.2085235586475127	1.0670595824306031	16.5242786307475207	T	T	T
6.1761685795667427	6.1379107040919614	15.0151768930644085	T	T	T
2.0649449643169349	7.1671442840291446	15.0579411285781042	T	T	T
2.0584115652536239	7.2059592956799170	12.2590327337071887	F	F	F
2.0585378094218574	2.0938343085271010	13.6963480075419053	F	F	F
2.0485827102933198	4.0538312459542984	16.2857818731221542	T	T	T
6.1801531386592492	4.1280190194280078	12.2955930440659973	F	F	F
3.4613798973919461	6.9080190651465747	18.9845604701622186	T	T	T
7.5783521997228451	5.1785096606659771	17.9276288714242469	T	T	T
7.5715355770031261	0.7768195463760293	17.6372397633756783	T	T	T
3.4532637643039044	3.1996939111031422	18.9720970810194594	T	T	T
4.7776751188475322	0.8895832147303342	17.7428773613420319	T	T	T
0.6289355840973120	3.2180851311756107	19.4552377235100167	T	T	T
0.7061975805488150	6.9435268240147945	19.0414573430000189	T	T	T
4.8737427391779775	5.1964782078596325	17.8606947491025316	T	T	T
6.2161571212958666	7.1338733332367292	19.0222517168782623	T	T	T
2.0280141811939809	0.9949210416329093	17.7217281467253436	T	T	T
2.0425330257834702	5.1063761698497938	17.7170353462753063	T	T	T
6.0369839511742169	3.0026880324813159	19.3223006670199275	T	T	T
0.7235872799205983	5.0296404830026811	19.0096435656394860	T	T	T
4.8203155638653001	7.0703196633387968	17.7961335448115854	T	T	T
3.4441742652108780	5.0228792321383011	18.8981143086683971	T	T	T
7.5937748613581464	7.1286499783680171	17.7765827637936482	T	T	T
4.6765711790855198	1.8404320207660663	19.2910956037776771	T	T	T
2.0764430737492847	7.3029357232324887	17.8971218524653324	T	T	T
1.9768053831728150	2.1767041853593074	19.0614795107976285	T	T	T
6.2311945314682964	4.0775251051657451	17.9225486952045934	T	T	T
3.0120617670639955	1.2486442271057208	20.2176064320111131	T	T	T
5.4587373563198280	0.8966501984461803	20.7818483992071101	T	T	T
2.1584627227260604	5.0653566874700644	20.3295767904402886	T	T	T
0.9122790062438751	0.2463597107534614	21.6118476620901738	T	T	T
2.0630876031678644	1.5639647275590915	23.6437406618225623	T	T	T
0.6877348842246328	0.1853587967341042	25.5195459337572643	T	T	T
0.5810939232362563	2.9283515166496024	21.5579588127898560	T	T	T
2.0236700375219749	4.3081348743466963	23.6328814535689844	T	T	T
0.6706862035865196	2.9308315246827790	25.5588435840305301	T	T	T
0.6390343910253742	5.7523528023318553	21.6429467819335954	T	T	T
2.1100240509636219	7.0657653152349464	23.6196596385300666	T	T	T
0.6816249837293731	5.6995493667957478	25.5308808193439276	T	T	T
3.6905572579791723	0.0251064963680388	21.7020420023761993	T	T	T
4.8569047185475407	1.5126453277758372	23.6341905268463712	T	T	T

```
  3.4731983711602563  0.1582093633658145 25.5514837936049624   T   T   T
  3.3708567109557532  2.9053753102811184 21.7346683311204991   T   T   T
  4.8101239325989491  4.2216673419141779 23.6357103831065736   T   T   T
  3.4270242159183253  2.9141526037233874 25.5680703079075471   T   T   T
  3.5312432123610455  5.6370166371181254 21.7167300669883829   T   T   T
  4.8782281907698186  6.9808376387332167 23.5649376433891220   T   T   T
  3.4424450851793820  5.6619721284649200 25.5569571007863487   T   T   T
  6.8607427931015517 -0.5052469596056363 20.7698844367830482   T   T   T
  7.5543643839261057  1.5459634163209344 23.5138271263390912   T   T   T
  6.2242608990839221  0.1439326768578549 25.5198740226553333   T   T   T
  6.1410563107840268  2.7803562571150553 21.4655816571455951   T   T   T
  7.5485558686881857  4.2695507533009129 23.6042133867135284   T   T   T
  6.1966741982151818  2.8892356344930481 25.5523564319594669   T   T   T
  6.1702879930692918  5.3803838971722548 21.5760074706520939   T   T   T
  7.5478906725351571  7.0782970110851444 23.4614940252921471   T   T   T
  6.1969231333239794  5.6555870959035541 25.5236146986996459   T   T   T
  2.0699624178438909  1.5446820301101249 27.4879773093073005   T   T   T
  0.7130478993580176  0.1754332667723511 29.4415294580478957   T   T   T
  2.0558196356499856  4.3020978708755555 27.4955734031961292   T   T   T
  0.6953556641394523  2.9245159355675039 29.4470555453202998   T   T   T
  2.0740713245544469  7.0462027618213954 27.4887023160922297   T   T   T
  0.6923729866198511  5.6745715192802795 29.4471402184057673   T   T   T
  4.8261833004496815  1.5264588484745278 27.4883997650742522   T   T   T
  3.4562212443649529  0.1638323198503881 29.4397235078739037   T   T   T
  4.8135550794403708  4.2796372883531104 27.4895528148931056   T   T   T
  3.4405856529905927  2.9130895982107528 29.4395144290832285   T   T   T
  4.8317341739899859  7.0263053339672830 27.4876882824059940   T   T   T
  3.4413967550693672  5.6617622612666549 29.4424655330114184   T   T   T
  7.5711310268946095  1.5360817422631208 27.4968011347083916   T   T   T
  6.2034923894211076  0.1575985547733947 29.4411589403888136   T   T   T
  7.5602744844320835  4.2937176835952515 27.4932298400404704   T   T   T
  6.1852611669472415  2.9052189706339209 29.4408972269985760   T   T   T
  7.5728862640508199  7.0379438324472092 27.4820046561082876   T   T   T
  6.1887350341973866  5.6518238199679418 29.4394635530084408   T   T   T

Oxide reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Pd E_tot= -710.87109812 eV
 D3-zero damping= -11.0932695 eV, D3-BJ damping= -16.5957909 eV
 O Al  O Al  O Al  H  O  H  O  H  O  H
 1.0000000000000000
     8.2439436957000023    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.2439436957000023    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.2904852797336304
  18  12  24  16  12   8   1   1   1   1   1   1   3
Selective dynamics
Cartesian
  3.3473887677478400  7.4003393451573807 10.9423958550990683   F   F   F
  7.5670196941003303  5.0589169937668892  9.3854545373318246   F   F   F
  3.3484015125796511  7.0420822184657137  8.0000187449185951   F   F   F
  3.4454253020583985  3.1798803951528498  8.1990827428381010   F   F   F
  7.4703600685588762  1.1967563746982413  9.5845317789161761   F   F   F
  3.4385096553888932  2.9913157022513954 10.8220669229527680   F   F   F
  0.6715507615048258  3.1799602445615576  8.1993257849376420   F   F   F
  4.8905134373423458  1.1966533309014900  9.5846030099037201   F   F   F
  0.6788447626099137  2.9911902342653081 10.8217845066302907   F   F   F
  0.7696156682374413  7.4004462040191576 10.9423584978630899   F   F   F
  4.7930268226572466  5.0590051461254415  9.3853700880230981   F   F   F
  0.7685065764046971  7.0418277978666568  8.0000000000000000   F   F   F
  6.1801705064822157  7.2225313263758544 10.9172067463060039   F   F   F
  6.1801274309999608  7.3293443642299252  8.0327436308783255   F   F   F
  2.0588097355269928  0.9093670483578636  9.5519775531218265   F   F   F
  2.0586976716953895  5.2755456603282509  9.4220834377914784   F   F   F
  6.1802620072973404  2.9631586676501263  8.1626394660302282   F   F   F
  6.1803440706559343  3.0658396473960003 10.8301543211852653   F   F   F
```

0.6189972349447344	5.0533416196151224	8.0560139425344559	F	F	F
4.7409971555249371	3.1855944447048308	9.5285274732362595	F	F	F
0.6473206805162403	1.1288536658996928	10.9191009939757393	F	F	F
7.6196682316059796	3.1855408931229516	9.5284873332419124	F	F	F
3.4695585581445858	1.1289144191539098	10.9192047381793671	F	F	F
3.4976874914628877	5.0532645383736545	8.0559839586400095	F	F	F
6.1800138965377762	1.0338453578144855	8.1168144920444938	F	F	F
6.1803794279467335	1.0330229471429531	10.8835529458276739	F	F	F
6.1800812184088922	6.1450085898655633	9.4463612987341499	F	F	F
2.0588797817143289	7.2048997704202415	9.4677862360962415	F	F	F
2.0585378094218574	2.0938343085271010	8.1383270166926529	F	F	F
2.0586483725600648	4.1105802756464582	10.8469192662674665	F	F	F
3.3499914254747680	7.3847103651630341	16.5159515599666484	T	T	T
7.5703689794049422	5.0276639439937227	14.9528618457606939	T	T	T
3.3484015125796511	7.0420822184657137	13.5580397357678457	F	F	F
7.5599425552607658	5.2473445396516336	12.3205669558782276	F	F	F
7.4690783348657828	0.8385288877277990	12.2001224306209899	F	F	F
3.4454253020583985	3.1798803951528498	13.7571037336873516	F	F	F
7.4568460489140298	1.2084494579559677	15.0921130335965898	T	T	T
3.4320325468385859	2.9562508135953625	16.3675149646869507	T	T	T
4.8912630981552843	0.8384497348568426	12.2001609218852387	F	F	F
0.6715507615048258	3.1799602445615576	13.7573467757868890	F	F	F
4.9011951515683752	1.2016862625256943	15.1489607158898512	T	T	T
0.6741239413917315	2.9355048918117665	16.3670061562620930	T	T	T
0.8074237006063103	7.3565512909171726	16.4463106756734021	T	T	T
4.7946963698425042	5.0349958819213656	14.9582520583675187	T	T	T
0.7685065764046971	7.0418277978666568	13.5580209908492506	F	F	F
4.8003683763421492	5.2472576311097123	12.3204488991888113	F	F	F
6.1521437135624009	7.1702833301974387	16.4641417525063538	T	T	T
6.1801274309999608	7.3293443642299252	13.5907646217275762	F	F	F
2.0584808851087932	1.0162421706238094	12.2256103096605884	F	F	F
2.0678752503170506	0.8907565982555583	15.0812858023824852	T	T	T
2.0638850658372192	5.2601175800666091	14.9504123058805209	T	T	T
2.0585644682872624	5.1728337497885555	12.3122395822918413	F	F	F
6.1802620072973404	2.9631586676501263	13.7206604568794788	F	F	F
6.1851643099907765	3.0693811960356396	16.3713081315061935	T	T	T
0.6189972349447344	5.0533416196151224	13.6140349333837065	F	F	F
4.7691316081237431	7.1097505399953924	12.2234202596149473	F	F	F
4.7542672327780515	3.1778882814925500	15.0746892631878531	T	T	T
0.6220433232183931	1.0678612957006020	16.3960761347559263	T	T	T
7.6084346885655041	3.1697825067587049	15.0661719694496679	T	T	T
3.4545417647507648	1.1058589662084930	16.4058778779516423	T	T	T
3.4976874914628877	5.0532645383736545	13.6140049494892601	F	F	F
7.5913184399609710	7.1098097820957546	12.2233730105456431	F	F	F
6.1800138965377762	1.0338453578144855	13.6748354828937444	F	F	F
6.2041502553385248	1.0790418275731908	16.5101767905173986	T	T	T
6.1884045879218315	6.1338071979761946	14.9870003961818838	T	T	T
2.0569510860346485	7.1693732325622737	15.0402460500303032	T	T	T
2.0584115652536239	7.2059592956799170	12.2590327337071869	F	F	F
2.0585378094218574	2.0938343085271010	13.6963480075419035	F	F	F
2.0400898789972239	4.0470358313603505	16.3007492359726243	T	T	T
6.1801531386592492	4.1280190194280078	12.2955930440659955	F	F	F
3.4415032509732884	6.9624081810373619	19.0286237546182520	T	T	T
7.5549091117432159	5.2271951190322881	17.9406460433777184	T	T	T
7.5639280276101779	0.7814154948984776	17.6408001799766261	T	T	T
3.3728489423570056	2.9425183102875443	19.3274803634478012	T	T	T
4.7936602690842740	0.9106422105713174	17.7250940824905925	T	T	T
0.5292388479377270	3.2658116639355885	19.4372464845206316	T	T	T
0.7093995307889286	6.9404652703510630	19.0461352216111877	T	T	T
4.7847569661733642	5.1278210812848206	17.9715076950785750	T	T	T
6.1335777249176466	7.1516603092171973	19.0230447769592566	T	T	T
2.0287408065903252	0.9980240860092952	17.7773219534880980	T	T	T
2.0797719546700386	5.0523732285659992	17.7865345831471302	T	T	T

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  6.1931158209028911  2.9999813509497968 19.2107718382244244   T   T   T
  0.7200985814198525  5.0947080912086404 19.0309943551150731   T   T   T
  4.8068735753665601  7.0014376156148064 17.7309960613500976   T   T   T
  3.3982722398082785  4.7496059687668373 18.9928940487390889   T   T   T
  7.5618867043533831  7.1545958132267717 17.8360116840318419   T   T   T
  4.8629270500290787  1.8939043069678325 19.2642314694600145   T   T   T
  2.0217313322458250  7.3244661511055966 17.8694561150813271   T   T   T
  1.8134493466800570  1.9920308429857367 19.2953507799397670   T   T   T
  6.2276341949532563  4.1018954247368198 17.8507318101649410   T   T   T
  7.7897351576232019  2.9611607618554325 19.4146718693268632   T   T   T
  1.7790517507679773  0.9137641890208312 20.6465332490502860   T   T   T
  1.2853837438440143  0.0811403622562567 20.5027607656262418   T   T   T
  4.7143315205107941  0.6757440738269298 20.5261528923880761   T   T   T
  4.0577323574642472  0.8363532049764203 21.2269623586176479   T   T   T
  2.1771400295379233  5.0898320427278323 20.3558799465307523   T   T   T
  2.1013954320884554  4.3941009644901357 21.0302958900361432   T   T   T
  3.6477026252304032  7.5660485652103446 19.7941113899099470   T   T   T
  5.9854074747132984  7.7448112450499327 19.7851548267461297   T   T   T

Metal reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Pd E_tot= -241.14571846 eV
 D3-zero damping= -19.5918853 eV, D3-BJ damping= -23.0696376 eV
Pd
 1.0000000000000000
     8.2439436957000023    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.2439436957000023    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
  0.0000260702354583  0.0000253164870683  7.9394162134360498
  1.3740224950001612  1.3740219999517895  9.8879526860300739
 -0.0007555027748666 -0.0007553210314964 11.8277878496272706
  1.3735230204547353  1.3735235440453020 13.7671311508483907
 -0.0006134116074896 -0.0006125273407870 15.7165509335488789
  0.0000829262048782  2.7469414356370878  7.9362752424037435
  1.3739589260942306  4.1217298404158571  9.8853145480320599
 -0.0005568469785369  2.7488852020360532 11.8275495198548803
  1.3736256489128775  4.1210731974257708 13.7699636105038543
 -0.0009262553542314  2.7460226014490225 15.7193906407008548
  0.0000703256072604  5.4970333926063137  7.9362414408117745
  1.3739170463673822  6.8693802362022653  9.8879992027111498
 -0.0006478136546837  5.4938219068163585 11.8277650854318370
  1.3735025021983005  6.8688712936691587 13.7673316204095659
 -0.0011058698326989  5.4960717494111995 15.7191221228160938
  2.7469422352906645  0.0000821601369144  7.9362749842730507
  4.1217303832602470  1.3739583024111033  9.8853144437964460
  2.7488852330069689 -0.0005567033428515 11.8275495623189713
  4.1210727914760827  1.3736261558616372 13.7699636011410682
  2.7460218423286133 -0.0009251267037524 15.7193907101769206
  2.7476440522837970  2.7476433550061166  7.9363581934679814
  4.1216969513983326  4.1216963411507557  9.8864411826469585
  2.7476975640546661  2.7476975478895658 11.8276553033336675
  4.1213931060324729  4.1213934361976188 13.7688289030204256
  2.7468293723854105  2.7468302469662200 15.7193751831893938
  2.7476085166823001  5.4964423728692644  7.9363257832051239
  4.1216550295233834  6.8694633660418623  9.8852635374483739
  2.7476155857506255  5.4952774768685853 11.8275926095212878
  4.1211652081322701  6.8690670581859719 13.7699183759514518
  2.7468301619621882  5.4954607412217191 15.7194848898295394
  5.4970341689909805  0.0000697163292463  7.9362412014308532
  6.8693806528400403  1.3739164984687962  9.8879990757863236
  5.4938217794753097 -0.0006478318721923 11.8277650968461696
  6.8688707135137301  1.3735029046411626 13.7673315813039885
  5.4960710199865730 -0.0011049428340850 15.7191219908006037
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  5.4964430624524558  2.7476077140000936  7.9363258764575964
  6.8694639299798634  4.1216543814411262  9.8852635633905237
  5.4952774309303134  2.7476154593871498 11.8275924987804846
  6.8690665982062598  4.1211655266152620 13.7699182310420607
  5.4954599947578924  2.7468307621626433 15.7194847303656804
  5.4964287021820946  5.4964279154529292  7.9363211725280891
  6.8693467658444751  6.8693463159645081  9.8879825686844001
  5.4951994316315060  5.4951993249332780 11.8275495111668221
  6.8687932008664188  6.8687936662934241 13.7673598354590645
  5.4953756322081713  5.4953761785839799 15.7196055569734430

Interface: 3O-g-Al2O3(110)/fcc(100)_3x3/Ni E_tot= -904.77147452 eV
 D3-zero damping= -28.9090129 eV, D3-BJ damping= -38.8118328 eV
 O Al  O Al  O Al  O Ni
 1.0000000000000000
     7.3615742453100017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.3615742453100017    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.3375309279805094
  18  12  24  16  12   8   3  45
Selective dynamics
Cartesian
  2.9891095634903047  6.6082629310387420 10.9423958550990701   F   F   F
  6.7571030746968939  4.5174487387511455  9.3854545373318263   F   F   F
  2.9900139117665812  6.2883509405641149  8.0000187449185969   F   F   F
  3.0766530078319358  2.8395300215761274  8.1990827428381028   F   F   F
  6.6707891652122342  1.0686646138163696  9.5845317789161779   F   F   F
  3.0704775597343890  2.6711478688010937 10.8220669229527697   F   F   F
  0.5996730415433136  2.8396013245073881  8.1993257849376437   F   F   F
  4.3670698267214378  1.0685725990491293  9.5846030099037218   F   F   F
  0.6061863478761169  2.6710358299603296 10.8217845066302925   F   F   F
  0.6872418215372981  6.6083583525352703 10.9423584978630917   F   F   F
  4.2800174427631861  4.5175274559472269  9.3853700880230999   F   F   F
  0.6862514385151685  6.2881237512238402  8.0000000000000018   F   F   F
  5.5186917465089316  6.4494861392522553 10.9172067463060056   F   F   F
  5.5186532815008631  6.5448667165043766  8.0327436308783273   F   F   F
  1.8384502956945641  0.8120352697479695  9.5519775531218283   F   F   F
  1.8383502263288560  4.7108911094681805  9.4220834377914802   F   F   F
  5.5187734537680928  2.6460045504578202  8.1626394660302299   F   F   F
  5.5188467336847689  2.7376953338840457 10.8301543211852671   F   F   F
  0.5527444474255763  4.5124701105267642  8.0560139425344577   F   F   F
  4.2335566381178262  2.8446324824335725  9.5285274732362613   F   F   F
  0.5780363653660630  1.0080296979642747 10.9191009939757411   F   F   F
  6.8041165105063817  2.8445846626084368  9.5284873332419142   F   F   F
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  3.1233214473221618  4.5124012794790360  8.0559839586400113   F   F   F
  5.5185518989097613  0.9231903613910094  8.1168144920444956   F   F   F
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  5.3186872928767537 -0.6685829628843799 25.8989158400857278   T   T   T
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  4.0851812878071296  5.4836511552000218 27.6568868268651684   T   T   T
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  6.5369109845246403  0.5816441046952083 27.6619369742706134   T   T   T
  5.2986413471692506 -0.6428564879951695 29.3745554097810846   T   T   T
  6.5325748761959215  3.0377035557156375 27.6695972879851553   T   T   T
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  6.5303768549447367  5.4824656466014154 27.6629906466572706   T   T   T
  5.2993371064909871  4.2696415422013976 29.3890251130313729   T   T   T

Oxide reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Ni E_tot= -680.23840985 eV
 D3-zero damping= -13.1589715 eV, D3-BJ damping= -20.0505747 eV
 O Al  O Al  O Al  H  O  H  O  H  O  H
 1.0000000000000000
     7.3615742453100017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.3615742453100017    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.2904852797336304
  18  12  24  16  12   8   1   1   1   1   1   1   3
Selective dynamics
Cartesian
  2.9891095634903047  6.6082629310387420 10.9423958550990683   F   F   F
  6.7571030746968939  4.5174487387511455  9.3854545373318246   F   F   F
  2.9900139117665812  6.2883509405641149  8.0000187449185951   F   F   F
  3.0766530078319358  2.8395300215761274  8.1990827428381010   F   F   F
  6.6707891652122342  1.0686646138163696  9.5845317789161761   F   F   F
  3.0704775597343890  2.6711478688010937 10.8220669229527680   F   F   F
  0.5996730415433136  2.8396013245073881  8.1993257849376420   F   F   F
  4.3670698267214378  1.0685725990491293  9.5846030099037201   F   F   F
  0.6061863478761169  2.6710358299603296 10.8217845066302907   F   F   F
  0.6872418215372981  6.6083583525352703 10.9423584978630899   F   F   F
  4.2800174427631861  4.5175274559472269  9.3853700880230981   F   F   F
  0.6862514385151685  6.2881237512238402  8.0000000000000000   F   F   F
  5.5186917465089316  6.4494861392522553 10.9172067463060039   F   F   F
  5.5186532815008631  6.5448667165043766  8.0327436308783255   F   F   F
  1.8384502956945641  0.8120352697479695  9.5519775531218265   F   F   F
  1.8383502263288560  4.7108911094681805  9.4220834377914784   F   F   F
  5.5187734537680928  2.6460045504578202  8.1626394660302282   F   F   F
  5.5188467336847689  2.7376953338840457 10.8301543211852653   F   F   F
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4.2335566381178262	2.8446324824335725	9.5285274732362595	F	F	F
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4.2586797914655738	6.3487765561898106	12.2234202596149473	F	F	F
4.1858268822581577	2.8564403550357849	15.1980832254305191	T	T	T
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3.1233214473221618	4.5124012794790360	13.6140049494892601	F	F	F
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1.8380947425590894	6.4346878535207148	12.2590327337071869	F	F	F
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0.4509480154319871	2.8440043798087773	20.3158230859988578	T	T	T
0.6381246948895140	6.3727486620487204	19.6150797722063608	T	T	T
4.3498545059644727	4.4192510904983529	18.3008761639676152	T	T	T
5.5146207631371089	6.8331709545911732	19.5582436236774981	T	T	T
1.8058534394152790	0.9270579494804265	18.1266373486255006	T	T	T
1.8435279952313481	4.4510531205636905	18.3702577392444404	T	T	T
5.5771401637963320	2.4924693424559852	19.7167787508745285	T	T	T

```
  0.6504838322868849  4.5310166375520025 19.7770578962055019   T   T   T
  4.2868552003695273  6.1897486299260542 18.0485399501907722   T   T   T
  3.2018740221242856  4.2282036664475102 19.5946882097546151   T   T   T
  6.7929416907257787  6.4435633660990392 18.2356371001906545   T   T   T
  4.4713967667628083  1.1274282104628508 19.8319128910205791   T   T   T
  1.8745865236202617  6.4092207842734208 18.2714620891926636   T   T   T
  1.5700346645367416  1.6274506356080058 19.7994734612105603   T   T   T
  5.7038015847044887  3.3342576423470640 18.1386940774533727   T   T   T
  6.5731029496342890  2.5284100384408594 20.1124030060819656   T   T   T
  1.7217829604648285  0.5667109874403087 21.3106362145142754   T   T   T
  1.4375698557207111 -0.3355361568897595 21.0006402245143207   T   T   T
  4.1797542993700700  0.7262827080594834 21.5884637868598723   T   T   T
  2.7656982879541689  0.5398176013576590 21.5744865002493498   T   T   T
  2.1124176490178801  4.6201577669536835 21.0637488001803135   T   T   T
  1.9945543794980132  3.8317039701696562 21.6266472391179612   T   T   T
  4.6483365626700088  7.3734656655869948 22.0430881802972785   T   T   T
  5.4418634749286063  6.1790895849728313 20.2693348108658427   T   T   T

Metal reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Ni E_tot= -244.01715482 eV
 D3-zero damping= -13.2341876 eV, D3-BJ damping= -16.2635305 eV
Ni
 1.0000000000000000
     7.3615742453100017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.3615742453100017    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
  0.0004044723896435  0.0004026210248400  8.3471906923878674
  1.2269986061066271  1.2269970502357732 10.0634831367242921
 -0.0010113053284333 -0.0010115841093046 11.8278685296456061
  1.2264990116897070  1.2265003707892768 13.5918019637391030
 -0.0012197526368572 -0.0012177708751624 15.3082548367556814
  0.0004044814728811  2.4542606822346364  8.3471913330323826
  1.2269985748844365  3.6808551750109459 10.0634832952082469
 -0.0010113053284333  2.4528464088150237 11.8278685506904377
  1.2264989755682421  3.6803585907575300 13.5918019410321165
 -0.0012198074449012  2.4526402759782462 15.3082545417281182
  0.0004045198270066  4.9081187896521250  8.3471910983843589
  1.2269985733671922  6.1347133394625537 10.0634831031465133
 -0.0010113445353290  4.9067047330828872 11.8278686209941135
  1.2264990390937287  6.1342168070718399 13.5918019958401590
 -0.0012197236819113  4.9064985677866755 15.3082545393075460
  2.4542625123275985  0.0004025766994193  8.3471911641293879
  3.6808566487708356  1.2269970110288779 10.0634832372571434
  2.4528466131422211 -0.0010115615976754 11.8278685022415768
  3.6803570492411999  1.2265003621418884 13.5918018229062074
  2.4526382573169325 -0.0012178198036691 15.3082547263490181
  2.4542625151650941  2.4542607228167346  8.3471910737279043
  3.6808566032629146  3.6808552275379598 10.0634833434309616
  2.4528466475509729  2.4528464153329348 11.8278685066543225
  3.6803570795141765  3.6803586322454591 13.5918018750091214
  2.4526382058136926  2.4526401887655154 15.3082543666592521
  2.4542625699731375  4.9081187821805008  8.3471911499512199
  3.6808566609084550  6.1347132846545120 10.0634832970771519
  2.4528465829130446  4.9067047308018559 11.8278686137028473
  3.6803570633251041  6.1342168113087201 13.5918018662606315
  2.4526382194082230  4.9064986172593059 15.3082545184623164
  4.9081206713838448  0.0004026172770151  8.3471911367680427
  6.1347149118139557  1.2269969954277291 10.0634832001119126
  4.9067048570726017 -0.0010115438210150 11.8278684771185887
  6.1342153505415125  1.2265004432486821 13.5918019011651836
  4.9064964386564318 -0.0012176232179926 15.3082544769188722
  4.9081207156658833  2.4542607311941915  8.3471915539079600
```

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  6.1347148570059122  3.6808552572230124 10.0634834125755610
  4.9067048633183461  2.4528464386296753 11.8278685228433940
  6.1342153120645806  3.6803586291910753 13.5918018662606315
  4.9064963647638153  2.4526403144117914 15.3082541801271041
  4.9081207156658833  4.9081188400429285  8.3471911892363782
  6.1347148592869427  6.1347133162954135 10.0634831209542295
  4.9067048359143248  4.9067047502211807 11.8278686046196100
  6.1342153431924071  6.1342168107956407 13.5918018936646590
  4.9064964683297312  4.9064986597512954 15.3082543001785929

Interface: 3O-g-Al2O3(110)/fcc(100)_3x3/Ir E_tot= -1086.7543796 eV
 D3-zero damping= -38.6003791 eV, D3-BJ damping= -45.3032455 eV
 O Al  O Al  O Al  O Ir
 1.0000000000000000
     8.1451896436500029    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1451896436500029    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.3375309279805094
  18  12  24  16  12   8   3  45
Selective dynamics
Cartesian
  3.3072904583944931  7.3116908143261332 10.9423958550990701   F   F   F
  7.4763745023913755  4.9983163188278228  9.3854545373318263   F   F   F
  3.3082910715743270  6.9577252432591177  8.0000187449185969   F   F   F
  3.4041526148381629  3.1417886655575238  8.1990827428381028   F   F   F
  7.3808727607516316  1.1824204517855503  9.5845317789161779   F   F   F
  3.3973198105747153  2.9554827856932442 10.8220669229527697   F   F   F
  0.6635062671094486  3.1418675584516125  8.1993257849376437   F   F   F
  4.8319300655521626  1.1823186423485719  9.5846030099037218   F   F   F
  0.6707128935075548  2.9553588206858872 10.8217845066302925   F   F   F
  0.7603964561024460  7.3117963931275423 10.9423584978630917   F   F   F
  4.7356112412567306  4.9984034152108698  9.3853700880230999   F   F   F
  0.7593006500606559  6.9574738703598040  8.0000000000000018   F   F   F
  6.1061383560451192  7.1360127545775418 10.9172067463060056   F   F   F
  6.1060957965632854  7.2415462809879134  8.0327436308783273   F   F   F
  2.0341472910358536  0.8984737569744050  9.5519775531218283   F   F   F
  2.0340365696148570  5.2123499945203990  9.4220834377914802   F   F   F
  6.1062287607736385  2.9276630436989151  8.1626394660302299   F   F   F
  6.1063098410967482  3.0291140098502445 10.8301543211852671   F   F   F
  0.6115822782911097  4.9928077319819257  8.0560139425344577   F   F   F
  4.6842048365635867  3.1474342666135295  9.5285274732362613   F   F   F
  0.6395664378216807  1.1153311483044748 10.9191009939757411   F   F   F
  7.5283923640208785  3.1473813565250790  9.5284873332419142   F   F   F
  3.4279967790872825  1.1153911737965609 10.9192047381793689   F   F   F
  3.4557887564234040  4.9927315740952523  8.0559839586400113   F   F   F
  6.1059836221283641  1.0214609430191108  8.1168144920444956   F   F   F
  6.1063447748432020  1.0206483839901006 10.8835529458276756   F   F   F
  6.1060501375520069  6.0713976433900552  9.4463612987341516   F   F   F
  2.0342164981411819  7.1185924067110227  9.4677862360962433   F   F   F
  2.0338786223286012  2.0687523053110657  8.1383270166926547   F   F   F
  2.0339878610329807  4.0613397090583305 10.8469192662674683   F   F   F
  3.3245269210984874  7.3016166091720045 16.4737708451359062   T   T   T
  7.4797256158718106  4.9777342763379480 14.9615687460165478   T   T   T
  3.3082910715743270  6.9577252432591177 13.5580397357678475   F   F   F
  7.4693821404696461  5.1844866945570187 12.3205669558782294   F   F   F
  7.3796063809232075  0.8284841653860766 12.2001224306209917   F   F   F
  3.4041526148381629  3.1417886655575238 13.7571037336873534   F   F   F
  7.3745005623335746  1.1943832320838437 15.0881783991387639   T   T   T
  3.3813115783982539  2.9173763076947883 16.3479540333948670   T   T   T
  4.8326707461918161  0.8284059606859262 12.2001609218852405   F   F   F
  0.6635062671094486  3.1418675584516125 13.7573467757868908   F   F   F
  4.8424085729430377  1.1801928055468713 15.1517198777642328   T   T   T
  0.6716212461270560  2.9141721787359671 16.3958599687456896   T   T   T
  0.7932984328695304  7.2432868638180175 16.4373144008267857   T   T   T
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4.7322485514251644	4.9799689957406441	14.9557972204421112	T	T	T
0.7593006500606559	6.9574738703598040	13.5580209908492524	F	F	F
4.7428648506031594	5.1844008270909452	12.3204488991888130	F	F	F
6.0840374726024438	7.1232914868834944	16.4722854878891418	T	T	T
6.1060957965632854	7.2415462809879134	13.5907646217275779	F	F	F
2.0338223799108510	1.0040686240886074	12.2256103096605901	F	F	F
2.0313454102084689	0.8776657374519501	15.0670800236975477	T	T	T
2.0406908235451127	5.1947408323135562	14.9483431889097975	T	T	T
2.0339049618479406	5.1108684680946661	12.3122395822918431	F	F	F
6.1062287607736385	2.9276630436989151	13.7206604568794805	F	F	F
6.1058786728489167	3.0095562259447775	16.4508310056183262	T	T	T
0.6115822782911097	4.9928077319819257	13.6140349333837083	F	F	F
4.7120022670648511	7.0245829671921678	12.2234202596149490	F	F	F
4.6976060086524489	3.1444696691906295	15.0994886008410827	T	T	T
0.6177124710884174	1.0525078213346333	16.3969990623292716	T	T	T
7.5205053576771093	3.1378221668259849	15.1027462415215101	T	T	T
3.4088439129492110	1.0805473838825892	16.3912581301721829	T	T	T
3.4557887564234040	4.9927315740952523	13.6140049494892619	F	F	F
7.5003821740159413	7.0246414996324837	12.2233730105456448	F	F	F
6.1059836221283641	1.0214609430191108	13.6748354828937462	F	F	F
6.1289136669776525	1.0568482836668549	16.5287753501270167	T	T	T
6.1043003149082784	6.0759885558609019	15.0168140139109187	T	T	T
2.0419586754070953	7.0837844909756180	15.0493455387862287	T	T	T
2.0337538904369699	7.1196392399368236	12.2590327337071887	F	F	F
2.0338786223286012	2.0687523053110657	13.6963480075419053	F	F	F
2.0245088394553976	4.0342644784313846	16.3406622411734190	T	T	T
6.1061211962709887	4.0785695544443232	12.2955930440659973	F	F	F
3.4219235167666184	6.8352195207992947	19.0147771786814630	T	T	T
7.4615439158666890	5.0826022827433279	17.9794387218321532	T	T	T
7.4850575975499902	0.7923588082168297	17.6421339238675010	T	T	T
3.3673333663582867	3.1395381768079718	19.0999568041427246	T	T	T
4.7127720349493067	0.8919733381183926	17.7622921967187537	T	T	T
0.5874698605727217	3.1243506712408866	19.6663481951866288	T	T	T
0.6903835327640854	6.8906521947755026	19.0083967761479968	T	T	T
4.8079001486785007	5.1027851790388068	17.9382669171923226	T	T	T
6.1535580626985062	7.1689673768579318	19.0033803805068864	T	T	T
2.0033880457138058	0.9807973142615430	17.7449032018936279	T	T	T
2.0029068488516892	5.0154245788156713	17.8193541210121005	T	T	T
5.9611146682029581	2.9292784663466196	19.4791260325562412	T	T	T
0.6491271530224544	4.9987856719028736	19.1124729339515724	T	T	T
4.7474108169195999	6.9615690839048883	17.7873449242182105	T	T	T
3.4068957213510007	4.9618295651513948	19.0142384762157057	T	T	T
7.5204016416303991	7.0425740053273165	17.7524893864429423	T	T	T
4.6220945070973363	1.7501696787076035	19.3593121667493548	T	T	T
2.0489583967097329	7.1813628292236826	17.8935918394472004	T	T	T
1.9012043175070961	2.0949584095317726	19.1320745977791198	T	T	T
6.1396923381630755	3.9637207074970484	18.0059001838544006	T	T	T
2.9848542213171334	1.1461275522478802	20.2592090197006023	T	T	T
5.3786707748215896	0.7375625767385352	20.8007737654945863	T	T	T
1.9807958678861965	5.1628693770686587	20.4263665871071929	T	T	T
0.5654703079823791	-0.0578571976224272	21.8530778511818831	T	T	T
1.8502142590969242	1.3045493644281003	23.6829390855191164	T	T	T
0.5015645172686193	-0.0811570693620478	25.5903667768611740	T	T	T
0.4917879099848360	2.6326091186385256	21.7511565164716743	T	T	T
1.8638408961438486	3.9834031913971049	23.6967033659009125	T	T	T
0.5260013771042701	2.6300809898757156	25.6128234408099367	T	T	T
0.4205580803312187	5.3776676622995208	21.8247225340637279	T	T	T
1.9063440227772641	6.7438920091296799	23.6988244256912601	T	T	T
0.5130194768402716	5.3610629057340136	25.5989317513759858	T	T	T
3.2943439001398214	-0.1329847561828928	21.8100639458220265	T	T	T
4.6090977056510223	1.2790797141049608	23.7095618308444749	T	T	T
3.2321287056740680	-0.0708860521765838	25.6038377080856705	T	T	T
3.2165999865682884	2.6489833546065769	21.8693749033715825	T	T	T

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  4.5814855387806928  3.9531759947316227 23.7011307579332140   T   T   T
  3.2384590114329144  2.6273615640847496 25.6498623160965131   T   T   T
  3.3537018289250753  5.3351281930753611 21.8701759512955078   T   T   T
  4.5847820076373118  6.7334330770305604 23.6810749247143804   T   T   T
  3.2431021849986426  5.3429211609407634 25.6069019121245667   T   T   T
  6.6378129751287336 -0.8319720034765592 20.8411259169376457   T   T   T
  7.2838353356833361  1.3127985614732636 23.6273680246416014   T   T   T
  5.9435082318520394 -0.0626672474889225 25.6051525667408306   T   T   T
  5.9210363195138864  2.6145367177768821 21.7026804627328893   T   T   T
  7.3135639562719668  3.9751852861250407 23.6794095872365240   T   T   T
  5.9516341049141319  2.6304597648863077 25.6074790304724580   T   T   T
  5.9193681445177049  5.2720476775725480 21.8935800195563566   T   T   T
  7.2763306273651382  6.7566632880805413 23.6541591951907471   T   T   T
  5.9771661378399026  5.3569558427053900 25.6052610749677925   T   T   T
  1.8735319615555215  1.2712370951952476 27.5637712005603639   T   T   T
  0.5220832340544537 -0.0803335914293010 29.3869928296109109   T   T   T
  1.8778004824548349  3.9951728613931929 27.5110003861094334   T   T   T
  0.5279978594196080  2.6485603752075408 29.3855666101331892   T   T   T
  1.8773448021940311  6.7137955565840661 27.5491110543871009   T   T   T
  0.5288232691196315  5.3404745603828729 29.3852181279668372   T   T   T
  4.5869672643423591  1.2798265087989498 27.5678088254892231   T   T   T
  3.2318097225252451 -0.0844056023088365 29.3875094771624248   T   T   T
  4.6046157352288448  4.0018985102245619 27.5593179936250152   T   T   T
  3.2271566471476074  2.6493173724650316 29.3815252645715006   T   T   T
  4.5988496946646658  6.7062521122103043 27.5525506116529719   T   T   T
  3.2249865365704946  5.3475607420350206 29.3779770975820611   T   T   T
  7.3140149115958595  1.2763776677771743 27.5550139712630724   T   T   T
  5.9534207040121929 -0.0771600603829108 29.3935144802227626   T   T   T
  7.3042392395279565  3.9866163040546732 27.5544861848331983   T   T   T
  5.9533654452906655  2.6367533217954180 29.3930139776321973   T   T   T
  7.3078419818259128  6.7111671255833922 27.5602784986786915   T   T   T
  5.9546246433989554  5.3534142567181906 29.3858539613000822   T   T   T

Oxide reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Ir E_tot= -710.80838817 eV
 D3-zero damping= -11.3560219 eV, D3-BJ damping= -16.9660715 eV
 O Al  O Al  O Al  H  O  H  O  H  O  H
 1.0000000000000000
     8.1451896436500029    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1451896436500029    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.2904852797336304
  18  12  24  16  12   8   1   1   1   1   1   1   3
Selective dynamics
Cartesian
  3.3072904583944931  7.3116908143261332 10.9423958550990683   F   F   F
  7.4763745023913755  4.9983163188278228  9.3854545373318246   F   F   F
  3.3082910715743270  6.9577252432591177  8.0000187449185951   F   F   F
  3.4041526148381629  3.1417886655575238  8.1990827428381010   F   F   F
  7.3808727607516316  1.1824204517855503  9.5845317789161761   F   F   F
  3.3973198105747153  2.9554827856932442 10.8220669229527680   F   F   F
  0.6635062671094486  3.1418675584516125  8.1993257849376420   F   F   F
  4.8319300655521626  1.1823186423485719  9.5846030099037201   F   F   F
  0.6707128935075548  2.9553588206858872 10.8217845066302907   F   F   F
  0.7603964561024460  7.3117963931275423 10.9423584978630899   F   F   F
  4.7356112412567306  4.9984034152108698  9.3853700880230981   F   F   F
  0.7593006500606559  6.9574738703598040  8.0000000000000000   F   F   F
  6.1061383560451192  7.1360127545775418 10.9172067463060039   F   F   F
  6.1060957965632854  7.2415462809879134  8.0327436308783255   F   F   F
  2.0341472910358536  0.8984737569744050  9.5519775531218265   F   F   F
  2.0340365696148570  5.2123499945203990  9.4220834377914784   F   F   F
  6.1062287607736385  2.9276630436989151  8.1626394660302282   F   F   F
  6.1063098410967482  3.0291140098502445 10.8301543211852653   F   F   F
  0.6115822782911097  4.9928077319819257  8.0560139425344559   F   F   F
  4.6842048365635867  3.1474342666135295  9.5285274732362595   F   F   F
```

0.6395664378216807	1.1153311483044748	10.9191009939757393	F	F	F
7.5283923640208785	3.1473813565250790	9.5284873332419124	F	F	F
3.4279967790872825	1.1153911737965609	10.9192047381793671	F	F	F
3.4557887564234040	4.9927315740952523	8.0559839586400095	F	F	F
6.1059836221283641	1.0214609430191108	8.1168144920444938	F	F	F
6.1063447748432020	1.0206483839901006	10.8835529458276739	F	F	F
6.1060501375520069	6.0713976433900552	9.4463612987341499	F	F	F
2.0342164981411819	7.1185924067110227	9.4677862360962415	F	F	F
2.0338786223286012	2.0687523053110657	8.1383270166926529	F	F	F
2.0339878610329807	4.0613397090583305	10.8469192662674665	F	F	F
3.3153354537267568	7.2813350521280817	16.5357331532159861	T	T	T
7.4857710748725586	4.9771103765963725	14.9635472234398357	T	T	T
3.3082910715743270	6.9577252432591177	13.5580397357678457	F	F	F
7.4693821404696461	5.1844866945570187	12.3205669558782276	F	F	F
7.3796063809232075	0.8284841653860766	12.2001224306209899	F	F	F
3.4041526148381629	3.1417886655575238	13.7571037336873516	F	F	F
7.3774577788276758	1.1793403478506184	15.1020805261030322	T	T	T
3.3940175809720734	2.9323576534364726	16.3878584064925050	T	T	T
4.8326707461918161	0.8284059606859262	12.2001609218852387	F	F	F
0.6635062671094486	3.1418675584516125	13.7573467757868890	F	F	F
4.8318559478606593	1.1750766238914523	15.1576284281800771	T	T	T
0.6639334386385657	2.9156068472618606	16.3863151512863539	T	T	T
0.7859209539059177	7.2558132127199473	16.4700334863470168	T	T	T
4.7322250258962768	4.9851294727224067	14.9685244802643691	T	T	T
0.7593006500606559	6.9574738703598040	13.5580209908492506	F	F	F
4.7428648506031594	5.1844008270909452	12.3204488991888113	F	F	F
6.0839786176589978	7.1022061311006919	16.4839953464751829	T	T	T
6.1060957965632854	7.2415462809879134	13.5907646217275762	F	F	F
2.0338223799108510	1.0040686240886074	12.2256103096605884	F	F	F
2.0410179927844427	0.8806425675905006	15.0958186539498964	T	T	T
2.0391261003445398	5.1997562753278928	14.9616549964807852	T	T	T
2.0339049618479406	5.1108684680946661	12.3122395822918413	F	F	F
6.1062287607736385	2.9276630436989151	13.7206604568794788	F	F	F
6.1104244062025579	3.0257419653016417	16.3815140479223409	T	T	T
0.6115822782911097	4.9928077319819257	13.6140349333837065	F	F	F
4.7120022670648511	7.0245829671921678	12.2234202596149473	F	F	F
4.6937162130411867	3.1400170229183879	15.0855864537230300	T	T	T
0.6188636059640680	1.0605939432392895	16.4218251264425810	T	T	T
7.5204278004224721	3.1316818442351653	15.0760567348006980	T	T	T
3.4083563220789053	1.0933403929424472	16.4318584245001773	T	T	T
3.4557887564234040	4.9927315740952523	13.6140049494892601	F	F	F
7.5003821740159413	7.0246414996324837	12.2233730105456431	F	F	F
6.1059836221283641	1.0214609430191108	13.6748354828937444	F	F	F
6.1289011883786069	1.0480302744481269	16.5157314303607663	T	T	T
6.1154364731909476	6.0786203841767303	15.0018920696163356	T	T	T
2.0297369100805422	7.0879889994658507	15.0477156230175044	T	T	T
2.0337538904369699	7.1196392399368236	12.2590327337071869	F	F	F
2.0338786223286012	2.0687523053110657	13.6963480075419035	F	F	F
2.0176130029900925	4.0289965255281404	16.3370431060034385	T	T	T
6.1061211962709887	4.0785695544443232	12.2955930440659955	F	F	F
3.4082389953712178	6.8606284237610202	19.0727365553845942	T	T	T
7.4752488159025638	5.1646663893396214	17.9547675768683348	T	T	T
7.4724318958693603	0.7948568400814130	17.6727978289736889	T	T	T
3.3303719358597603	2.9154721839126641	19.3614938853365786	T	T	T
4.7351087486756889	0.8927407230956111	17.7531798271863082	T	T	T
0.5020334626182664	3.2212000728173797	19.4884734314863977	T	T	T
0.6974359900855556	6.8770985395609125	19.0963243279573867	T	T	T
4.7272892520416967	5.0581562754453095	17.9791774452019837	T	T	T
6.0654899037516969	7.0569137312465227	19.0611746886088795	T	T	T
2.0072326073424640	0.9812788944602950	17.8034812626049117	T	T	T
2.0514898584745231	5.0236146285707743	17.8299801703319147	T	T	T
6.1326157837552602	2.9619103170994419	19.2487055710333514	T	T	T
0.6975306561176821	5.0355525121509128	19.0936515603687020	T	T	T

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  4.7522765889184315  6.9209616182503675 17.7557970931087432   T   T   T
  3.3673098647375941  4.7242584986826870 19.0500489227095571   T   T   T
  7.4772670762283679  7.0761574930203555 17.8640211499450885   T   T   T
  4.8040686150340406  1.8572562415346696 19.3017932738002287   T   T   T
  1.9983712131918001  7.1994131469682925 17.8874677092227046   T   T   T
  1.7779787346594200  1.9571588346735211 19.3279310358431289   T   T   T
  6.1607116744935499  4.0364448127937784 17.8633356994242938   T   T   T
  7.6485744509837419  2.9236518072196529 19.4586572736089956   T   T   T
  1.7723636416217183  0.8821240732882710 20.6851771862802920   T   T   T
  1.2957116045244730  0.0399756495388157 20.5288345003798689   T   T   T
  4.6274752765321230  0.6524096994434164 20.5736119401578144   T   T   T
  3.8810892968288675  0.7979270711553823 21.1884239829655172   T   T   T
  2.1411783567664862  5.0338790839526517 20.4203261150211688   T   T   T
  2.0668207395970288  4.3150946587622458 21.0707511164353889   T   T   T
  3.6333379817996612  7.4804934986814331 19.8251812284993534   T   T   T
  5.9221538065730135  7.6411391012035796 19.8295572920663794   T   T   T

Metal reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Ir E_tot= -398.20657225 eV
 D3-zero damping= -23.8108995 eV, D3-BJ damping= -25.0242167 eV
Ir
 1.0000000000000000
     8.1451896436500029    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1451896436500029    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0002798442392654 -0.0002800191392171  8.0568916680494471
  1.3571590845927890  1.3571588741174361  9.8876191036087384
 -0.0004570447348009 -0.0004570792896131 11.8276015897431694
  1.3567566149253463  1.3567566950342165 13.7678490544673018
 -0.0007900565755808 -0.0007899466945541 15.5987926047195593
 -0.0002447812562515  2.7147740414621095  8.0569498530224415
  1.3571773460458718  4.0722852325851413  9.8874382930875395
 -0.0005077959345058  2.7145956018077748 11.8276045481942305
  1.3568613442787136  4.0719230501926766 13.7679664692265629
 -0.0006574622226124  2.7143669859322759 15.5985915135074116
 -0.0002492176801693  5.4299021328385777  8.0569530400386764
  1.3571523202601914  6.7874010974721539  9.8876170503683269
 -0.0004558803362309  5.4296442635444535 11.8275931755308665
  1.3567376737905583  6.7870777241239129 13.7678076910423357
 -0.0007125651108604  5.4294527739395564 15.5985739600482276
  2.7147741916988752 -0.0002449183364295  8.0569499721699653
  4.0722853195967614  1.3571770949336159  9.8874382940801127
  2.7145955558505817 -0.0005077899224245 11.8276045431862382
  4.0719228018809090  1.3568613940624581 13.7679664675800293
  2.7143668063372686 -0.0006573716379037 15.5985914384189535
  2.7148113971455019  2.7148111992662107  8.0567322342520811
  4.0722692999470009  4.0722691822375356  9.8872815348782179
  2.7147368722918559  2.7147368919566386 11.8276880311105366
  4.0719974933628835  4.0719977356538388 13.7680120065208023
  2.7144139561738374  2.7144141675377296 15.5988616156143980
  2.7148104483069764  5.4298735870089443  8.0567381312202802
  4.0722729116345207  6.7873279190569091  9.8874241432959273
  2.7146653960081664  5.4294899827352427 11.8277012333384199
  4.0719140696564100  6.7869936366617933 13.7679517320240219
  2.7143946899100384  5.4294822092805894 15.5988122176703783
  5.4299022925957718 -0.0002493437176963  8.0569529909489361
  6.7874012111253652  1.3571521190212568  9.8876170569754738
  5.4296441759375380 -0.0004559109540933 11.8275931440159088
  6.7870776273913380  1.3567376957423669 13.7678076724008047
  5.4294526067121742 -0.0007124623355347 15.5985739652085353
  5.4298737407453217  2.7148103015978364  8.0567380103415385
  6.7873281168755888  4.0722727728664161  9.8874241203196718
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  5.4294899296723536  2.7146654085973214 11.8277012392916063
  6.7869935307697284  4.0719142616346451 13.7679517147750943
  5.4294820443910066  2.7143949456707785 15.5988122511544454
  5.4298794157802135  5.4298791899920724  8.0567296777420641
  6.7874025853856468  6.7874023679117830  9.8876198588143431
  5.4295140362835497  5.4295140352521711 11.8276428900953263
  6.7870469000109042  6.7870470153464648 13.7677651371691852
  5.4294266363748367  5.4294267474240847 15.5988587611836493

Interface: 3O-g-Al2O3(110)/fcc(100)_3x3/Rh E_tot= -1014.65343847 eV
 D3-zero damping= -34.4479392 eV, D3-BJ damping= -42.9652144 eV
 O Al  O Al  O Al  O Rh
 1.0000000000000000
     8.0329880858400013    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.0329880858400013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.3375309279805094
  18  12  24  16  12   8   3  45
Selective dynamics
Cartesian
  3.2617318946535843  7.2109708635964349 10.9423958550990701   F   F   F
  7.3733860021060238  4.9294635478138478  9.3854545373318263   F   F   F
  3.2627187241939386  6.8618812365187392  8.0000187449185969   F   F   F
  3.3572597562163131  3.0985099209232376  8.1990827428381028   F   F   F
  7.2791998153709958  1.1661323820804854  9.5845317789161779   F   F   F
  3.3505210751490235  2.9147704404756039 10.8220669229527697   F   F   F
  0.6543663403498037  3.0985877270524989  8.1993257849376437   F   F   F
  4.7653692972578847  1.1660319750881312  9.5846030099037218   F   F   F
  0.6614736940797710  2.9146481831101250 10.8217845066302925   F   F   F
  0.7499218483080882  7.2110749880294982 10.9423584978630917   F   F   F
  4.6703772833382917  4.9295494444274253  9.3853700880230999   F   F   F
  0.7488411372058054  6.8616333263295806  8.0000000000000018   F   F   F
  6.0220251228700281  7.0377128029932523 10.9172067463060056   F   F   F
  6.0219831496532619  7.1417925847294708  8.0327436308783273   F   F   F
  2.0061265198992171  0.8860971077379413  9.5519775531218283   F   F   F
  2.0060173236871433  5.1405488683560643  9.4220834377914802   F   F   F
  6.0221142822559814  2.8873339207911530  8.1626394660302299   F   F   F
  6.0221942456820070  2.9873873803230535 10.8301543211852671   F   F   F
  0.6031576144888678  4.9240308428138597  8.0560139425344577   F   F   F
  4.6196790117814324  3.1040777527361723  9.5285274732362613   F   F   F
  0.6307562868262977  1.0999672466903065 10.9191009939757411   F   F   F
  7.4246873076620501  3.1040255714943914  9.5284873332419142   F   F   F
  3.3807754625055231  1.1000264453196658 10.9192047381793689   F   F   F
  3.4081845999952867  4.9239557340167588  8.0559839586400113   F   F   F
  6.0218725204428107  1.0073901215818017  8.1168144920444956   F   F   F
  6.0222286982093678  1.0065887557100852 10.8835529458276756   F   F   F
  6.0219381196036679  5.9877629702301212  9.4463612987341516   F   F   F
  2.0061947736633257  7.0205324237774009  9.4677862360962433   F   F   F
  2.0058615521552090  2.0402548434306178  8.1383270166926547   F   F   F
  2.0059692860753731  4.0053939715017819 10.8469192662674683   F   F   F
  3.2778530215499249  7.1813522320913226 16.5052535382762144   T   T   T
  7.3840474405773984  4.9235602596863810 14.9722623524881620   T   T   T
  3.2627187241939386  6.8618812365187392 13.5580397357678475   F   F   F
  7.3664899613179591  5.1130693907219849 12.3205669558782294   F   F   F
  7.2779508801688779  0.8170716362683897 12.2001224306209917   F   F   F
  3.3572597562163131  3.0985099209232376 13.7571037336873534   F   F   F
  7.2798113703934577  1.1608056076936430 15.1020024255093475   T   T   T
  3.3349617330188068  2.8916891587973206 16.3714722580839869   T   T   T
  4.7660997748789171  0.8169945088530625 12.2001609218852405   F   F   F
  0.6543663403498037  3.0985877270524989 13.7573467757868908   F   F   F
  4.7634110897274153  1.1520306393089519 15.1603626620007663   T   T   T
  0.6563702123297859  2.8885511774446080 16.4165232922658539   T   T   T
  0.7641596381837692  7.1287145743122489 16.4868486929341458   T   T   T
  4.6607419144593552  4.9264541875068728 14.9663136161092538   T   T   T
```

0.7488411372058054	6.8616333263295806	13.5580209908492524	F	F	F
4.6775309728174106	5.1129847060968121	12.3204488991888130	F	F	F
6.0021119642604930	7.0418643940888082	16.5080935549645496	T	T	T
6.0219831496532619	7.1417925847294708	13.5907646217275779	F	F	F
2.0058060844876073	0.9902373851979678	12.2256103096605901	F	F	F
1.9973628268232753	0.8623705796322976	15.0803983908706432	T	T	T
2.0100963714111777	5.1228534344418239	14.9565290674608402	T	T	T
2.0058875288425910	5.0404652695234331	12.3122395822918431	F	F	F
6.0221142822559814	2.8873339207911530	13.7206604568794805	F	F	F
6.0211192779172418	2.9724915565570234	16.4534136829194964	T	T	T
0.6031576144888678	4.9240308428138597	13.6140349333837083	F	F	F
4.6470935273179368	6.9278179824138180	12.2234202596149490	F	F	F
4.6288393559231515	3.1052205891127826	15.1135213413946321	T	T	T
0.6054423357079887	1.0370894426343265	16.4198691483113066	T	T	T
7.4180194290113866	3.0981306015175036	15.1138046592622501	T	T	T
3.3546393904569696	1.0635396556245269	16.4134670350527117	T	T	T
3.4081845999952867	4.9239557340167588	13.6140049494892619	F	F	F
7.3970629634250580	6.9278757085584823	12.2233730105456448	F	F	F
6.0218725204428107	1.0073901215818017	13.6748354828937462	F	F	F
6.0390244302570411	1.0336410556252278	16.5427524833965514	T	T	T
6.0214722003032328	6.0186425660065836	15.0428439241200138	T	T	T
2.0087467789124123	6.9846577171610083	15.0712330419106877	T	T	T
2.0057385384694340	7.0215648366736776	12.2590327337071887	F	F	F
2.0058615521552090	2.0402548434306178	13.6963480075419053	F	F	F
1.9934382283767522	4.0118346605988799	16.3728454755607657	T	T	T
6.0220081994750956	4.0223864724455067	12.2955930440659973	F	F	F
3.3777100263457869	6.7612082399892444	19.0788975754617063	T	T	T
7.3635415826414610	5.0288739150884654	18.0108914572934538	T	T	T
7.3776918404973602	0.8148222206215238	17.6871996359604395	T	T	T
3.3017512466111176	3.0867505976431659	19.1379509383454369	T	T	T
4.6382890857497854	0.8812542410497793	17.7871626704529469	T	T	T
0.5323114099022627	3.1046375461246853	19.6767728437200695	T	T	T
0.6704265469286282	6.8275367057920393	19.1180404371830726	T	T	T
4.7304234162725978	5.0254828050597062	17.9549390510214799	T	T	T
6.0514033183923912	7.0650657844894420	19.0715386445606079	T	T	T
1.9718024349889933	0.9666573018433511	17.7597309772863028	T	T	T
1.9671559960537737	4.9878680666120765	17.8522613175423501	T	T	T
5.8654198726885118	2.8720553145845487	19.4930072930387439	T	T	T
0.6370686743417682	4.9277480391538369	19.1721623802788415	T	T	T
4.6830136119637515	6.8764922244845152	17.8344169757962128	T	T	T
3.3580038678402966	4.8951306031248372	19.0592465698205835	T	T	T
7.4012998217085251	6.9619592057095705	17.8275268611566702	T	T	T
4.5187090256796445	1.7034748688079326	19.3938603705223187	T	T	T
2.0134903087710558	7.0676144734581063	17.9366602376029718	T	T	T
1.8215497245286318	2.0631825881574049	19.1447702677052547	T	T	T
6.0608530093307182	3.8899571156077801	18.0243975119878392	T	T	T
2.8212724151502262	1.1227053164667675	20.3174424490427192	T	T	T
5.1929510042120306	0.7226130728836815	20.8835418123048626	T	T	T
2.0112541312413286	5.0434805186292726	20.4619758896195698	T	T	T
0.6305824870586465	-0.0351842946630576	21.7996267024063251	T	T	T
1.8528494795419450	1.2993895695114772	23.6661980950140141	T	T	T
0.5281783567765044	-0.0628711416635957	25.5433297174459177	T	T	T
0.4772998901241878	2.6353190163815237	21.7485419644866411	T	T	T
1.8733301233720367	3.9453556385536048	23.7079353032323539	T	T	T
0.5405497460457076	2.6114108689764319	25.5716404068930920	T	T	T
0.4819345028200758	5.3103854407296360	21.8454074706402608	T	T	T
1.9189175688428948	6.6784536972748150	23.6900317876907742	T	T	T
0.5443643006588059	5.2986127912872085	25.5674873192841474	T	T	T
3.3730629583853506	-0.1229576403192313	21.8081793124184813	T	T	T
4.5760853288440630	1.2796158907843347	23.6983784504598418	T	T	T
3.2288855725379522	-0.0545760857929336	25.5636848180740124	T	T	T
3.1714692204742141	2.6292103398468205	21.8585593745870526	T	T	T
4.5561540999887216	3.9210555861291492	23.6926545800444615	T	T	T

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  3.2256343612308394  2.6090007973904905 25.5929933621215469   T   T   T
  3.3371959086852137  5.2805919602734335 21.9069757446400608   T   T   T
  4.5802530668995276  6.6451516350244502 23.6675890713138415   T   T   T
  3.2326607602893751  5.2940447585657946 25.5678647456413728   T   T   T
  6.5265018629567493 -0.7460390675832930 20.9021554819011399   T   T   T
  7.2177522298634953  1.2911683949702477 23.5938876373368522   T   T   T
  5.9014794099228807 -0.0426854510026210 25.5630063362215765   T   T   T
  5.8787393731381217  2.5803218847679195 21.6706900876685502   T   T   T
  7.2457991052043660  3.9465882786650344 23.6757168794887782   T   T   T
  5.9067564634550109  2.6049227946362215 25.5618888223293581   T   T   T
  5.8757235296721824  5.1794548530710145 21.8709678703402197   T   T   T
  7.2282600414584044  6.6751750685758982 23.6184783176886128   T   T   T
  5.9405692911380479  5.2968316206418349 25.5718804016233534   T   T   T
  1.8792708819910757  1.2695634532048972 27.4762812505648810   T   T   T
  0.5509371164615900 -0.0631560004661711 29.3119037171724877   T   T   T
  1.8893099481105458  3.9550888609158097 27.4414559818357162   T   T   T
  0.5518077491918851  2.6222160708366857 29.3026206963240377   T   T   T
  1.8852417786307145  6.6422596352748657 27.4645442003146520   T   T   T
  0.5599373299268577  5.2862541524280351 29.3085244481451603   T   T   T
  4.5607823460908223  1.2787976482890011 27.4881385103524565   T   T   T
  3.2231121130852722 -0.0676447615137526 29.3049468602801930   T   T   T
  4.5792189080886034  3.9636280835722419 27.4766349767732727   T   T   T
  3.2193677107021488  2.6238651873077141 29.2954855717549307   T   T   T
  4.5760491718084557  6.6303268020373380 27.4684592676213413   T   T   T
  3.2218071757678421  5.2915933036018892 29.2907147982293843   T   T   T
  7.2476477943014945  1.2704573573371483 27.4773944428801506   T   T   T
  5.9042862438339370 -0.0595249064798568 29.3145845376912106   T   T   T
  7.2419028013252857  3.9474551490415211 27.4813268669908730   T   T   T
  5.9108092172080680  2.6174178828194132 29.3141333780157680   T   T   T
  7.2433791729486892  6.6360237403406250 27.4838941263693322   T   T   T
  5.9042835448361668  5.2978437214971796 29.3102244580067968   T   T   T

Oxide reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Rh E_tot= -709.86681628 eV
 D3-zero damping= -11.6461192 eV, D3-BJ damping= -17.3914056 eV
 O Al  O Al  O Al  H  O  H  O  H  O  H
 1.0000000000000000
     8.0329880858400013    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.0329880858400013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.2904852797336304
  18  12  24  16  12   8   1   1   1   1   1   1   3
Selective dynamics
Cartesian
  3.2617318946535843  7.2109708635964349 10.9423958550990683   F   F   F
  7.3733860021060238  4.9294635478138478  9.3854545373318246   F   F   F
  3.2627187241939386  6.8618812365187392  8.0000187449185951   F   F   F
  3.3572597562163131  3.0985099209232376  8.1990827428381010   F   F   F
  7.2791998153709958  1.1661323820804854  9.5845317789161761   F   F   F
  3.3505210751490235  2.9147704404756039 10.8220669229527680   F   F   F
  0.6543663403498037  3.0985877270524989  8.1993257849376420   F   F   F
  4.7653692972578847  1.1660319750881312  9.5846030099037201   F   F   F
  0.6614736940797710  2.9146481831101250 10.8217845066302907   F   F   F
  0.7499218483080882  7.2110749880294982 10.9423584978630899   F   F   F
  4.6703772833382917  4.9295494444274253  9.3853700880230981   F   F   F
  0.7488411372058054  6.8616333263295806  8.0000000000000000   F   F   F
  6.0220251228700281  7.0377128029932523 10.9172067463060039   F   F   F
  6.0219831496532619  7.1417925847294708  8.0327436308783255   F   F   F
  2.0061265198992171  0.8860971077379413  9.5519775531218265   F   F   F
  2.0060173236871433  5.1405488683560643  9.4220834377914784   F   F   F
  6.0221142822559814  2.8873339207911530  8.1626394660302282   F   F   F
  6.0221942456820070  2.9873873803230535 10.8301543211852653   F   F   F
  0.6031576144888678  4.9240308428138597  8.0560139425344559   F   F   F
  4.6196790117814324  3.1040777527361723  9.5285274732362595   F   F   F
  0.6307562868262977  1.0999672466903065 10.9191009939757393   F   F   F
```

7.4246873076620501	3.1040255714943914	9.5284873332419124	F	F	F
3.3807754625055231	1.1000264453196658	10.9192047381793671	F	F	F
3.4081845999952867	4.9239557340167588	8.0559839586400095	F	F	F
6.0218725204428107	1.0073901215818017	8.1168144920444938	F	F	F
6.0222286982093678	1.0065887557100852	10.8835529458276739	F	F	F
6.0219381196036679	5.9877629702301212	9.4463612987341499	F	F	F
2.0061947736633257	7.0205324237774009	9.4677862360962415	F	F	F
2.0058615521552090	2.0402548434306178	8.1383270166926529	F	F	F
2.0059692860753731	4.0053939715017819	10.8469192662674665	F	F	F
3.2759866542906537	7.1660459874426010	16.5628607366788110	T	T	T
7.3900521980456286	4.9208389236572003	14.9752495907569880	T	T	T
3.2627187241939386	6.8618812365187392	13.5580397357678457	F	F	F
7.3664899613179591	5.1130693907219849	12.3205669558782276	F	F	F
7.2779508801688779	0.8170716362683897	12.2001224306209899	F	F	F
3.3572597562163131	3.0985099209232376	13.7571037336873516	F	F	F
7.2867747892780850	1.1472566464875871	15.1147326008507417	T	T	T
3.3522353675680923	2.9036158677449739	16.4117861842982187	T	T	T
4.7660997748789171	0.8169945088530625	12.2001609218852387	F	F	F
0.6543663403498037	3.0985877270524989	13.7573467757868890	F	F	F
4.7551990354090430	1.1438379769350659	15.1703358821736387	T	T	T
0.6501655734583702	2.8913678728655854	16.4114322996050426	T	T	T
0.7675737448348954	7.1426043995839548	16.5018516415439898	T	T	T
4.6602988762685245	4.9293232677831469	14.9797978424754916	T	T	T
0.7488411372058054	6.8616333263295806	13.5580209908492506	F	F	F
4.6775309728174106	5.1129847060968121	12.3204488991888113	F	F	F
6.0073556618773702	7.0144456161713595	16.5124715809233287	T	T	T
6.0219831496532619	7.1417925847294708	13.5907646217275762	F	F	F
2.0058060844876073	0.9902373851979678	12.2256103096605884	F	F	F
2.0118328636654605	0.8700119101129561	15.1136089654697692	T	T	T
2.0114580667744062	5.1274036307780948	14.9755658581433231	T	T	T
2.0058875288425910	5.0404652695234331	12.3122395822918413	F	F	F
6.0221142822559814	2.8873339207911530	13.7206604568794788	F	F	F
6.0260341259054453	2.9794976172687950	16.3911566786111216	T	T	T
0.6031576144888678	4.9240308428138597	13.6140349333837065	F	F	F
4.6470935273179368	6.9278179824138180	12.2234202596149473	F	F	F
4.6238802712560716	3.0982195215213459	15.0975021708448285	T	T	T
0.6154873597203596	1.0505620303809182	16.4518858667036803	T	T	T
7.4219779461358586	3.0895470890676995	15.0874487332302341	T	T	T
3.3586583549003803	1.0787071881474264	16.4618169882179224	T	T	T
3.4081845999952867	4.9239557340167588	13.6140049494892601	F	F	F
7.3970629634250580	6.9278757085584823	12.2233730105456431	F	F	F
6.0218725204428107	1.0073901215818017	13.6748354828937444	F	F	F
6.0445823894477648	1.0210773607827666	16.5267205018897485	T	T	T
6.0319158142790190	6.0171495807322097	15.0203721264474961	T	T	T
1.9996465479636085	6.9922903318687650	15.0599913904090652	T	T	T
2.0057385384694340	7.0215648366736776	12.2590327337071869	F	F	F
2.0058615521552090	2.0402548434306178	13.6963480075419035	F	F	F
1.9912681430204395	4.0051848790053644	16.3809374252143023	T	T	T
6.0220081994750956	4.0223864724455067	12.2955930440659955	F	F	F
3.3743467578013897	6.7591264816882450	19.1263205519322703	T	T	T
7.3916063601960174	5.0881654215061154	17.9742612991333210	T	T	T
7.3691867817653689	0.8067923177303375	17.7091592598497840	T	T	T
3.2848388270579667	2.8748941734856213	19.4163351326116889	T	T	T
4.6708486745328681	0.8743994744202305	17.7894175158448036	T	T	T
0.4738634992680460	3.1728531410227663	19.5637724096679584	T	T	T
0.6868692462848417	6.8018367808051474	19.1533750739720681	T	T	T
4.6645254572114707	4.9774413451969606	17.9992983757669052	T	T	T
5.9931555170514637	6.9481574291434027	19.1083799875291831	T	T	T
1.9825101918699024	0.9686108668359238	17.8393719480976962	T	T	T
2.0262686868510613	4.9711418261921487	17.8880483255412130	T	T	T
6.0613812508743727	2.9160582203009366	19.2907331557823198	T	T	T
0.6798118174122807	4.9665789902738009	19.1669773943324913	T	T	T
4.6924753839794953	6.8267184698477550	17.7902863622265777	T	T	T

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  3.3376673284817917  4.6794702611374976 19.1201620448579277   T   T   T
  7.3836453709677654  6.9821826676856116 17.8960851922646604   T   T   T
  4.7394252241048465  1.8082459464714542 19.3516774693555504   T   T   T
  1.9768114893545974  7.0761164289181853 17.9200817289231296   T   T   T
  1.7356095622756122  1.9168613441825302 19.3783611129591407   T   T   T
  6.0878710065670507  3.9612322424487334 17.8786038503663072   T   T   T
  7.4862008285457167  2.8833436575703923 19.5197936898761135   T   T   T
  1.7510401445468400  0.8458476816173717 20.7403901257587364   T   T   T
  1.2884873169372975 -0.0028559099891758 20.5689541708009429   T   T   T
  4.5492884096898036  0.6218985273378108 20.6395211058712853   T   T   T
  3.7524156792366274  0.7649721586603032 21.1956546132243986   T   T   T
  2.1148679468640741  4.9777067083724047 20.4967771387773858   T   T   T
  2.0400175521393695  4.2487208799909606 21.1358567701508875   T   T   T
  3.6218332470557781  7.3848962024459768 19.8731675866270017   T   T   T
  5.8641331852795293  7.5190151687913893 19.8878174248985218   T   T   T

Metal reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Rh E_tot= -327.12330447 eV
 D3-zero damping= -19.3210663 eV, D3-BJ damping= -22.4126897 eV
Rh
 1.0000000000000000
     8.0329880858400013    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.0329880858400013    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0003155027487574 -0.0003133579117291  8.0889891459620102
  1.3384376326513099  1.3384348145679728  9.9206979029047417
 -0.0008827891331823 -0.0008721075381926 11.8276838387698184
  1.3381977302843577  1.3381892973316925 13.7354434410448221
 -0.0006629120124709 -0.0006653430154914 15.5664906175198148
 -0.0001827917914599  2.6772966337827211  8.0915786761431772
  1.3385323974649270  4.0159180678141553  9.9215091613356847
 -0.0004278480714868  2.6761657572115851 11.8278684661890452
  1.3381419333702242  4.0158083854955953 13.7343079870090357
 -0.0003845355450809  2.6770518128987950 15.5639950898660100
 -0.0002346758408553  5.3550103640989803  8.0915768074533538
  1.3382884564314419  6.6936492816352899  9.9202506299082991
 -0.0006174111265524  5.3550222982432585 11.8274410088403421
  1.3383385090992137  6.6930358014614244 13.7352239141672055
 -0.0005649400981955  5.3545502203519684 15.5637808782028202
  2.6773112541004394 -0.0000611861572501  8.0915860762173626
  4.0159302255602833  1.3385292031710490  9.9215011901375227
  2.6761504294973029 -0.0004843855502316 11.8278763389795696
  4.0158106158183093  1.3381294703497566 13.7342909772195103
  2.6770485662973624 -0.0003839734108014 15.5639974445102975
  2.6777192802994536  2.6777220264064590  8.0909390338675315
  4.0161489801522956  4.0161519492249225  9.9224563858999257
  2.6771031681837862  2.6770697464533004 11.8274728524137309
  4.0158852187421417  4.0158787935051938 13.7330191220469189
  2.6774358118276647  2.6774255670120919 15.5642436815892733
  2.6775840561348270  5.3548696572205063  8.0909809497277987
  4.0159225128538356  6.6941789222509671  9.9214783067905827
  2.6770689196694577  5.3551935152785326 11.8277164449983161
  4.0156832575488508  6.6942304620168551 13.7341352421476000
  2.6773731206987326  5.3547778135191804 15.5642196151160075
  5.3550205699767996 -0.0002258472658032  8.0915784266744240
  6.6936486610207355  1.3382985585550145  9.9202589850943230
  5.3550222543762773 -0.0006087393603481 11.8274411460925286
  6.6930444516733729  1.3383479137121488 13.7352182647289407
  5.3545537018615983 -0.0005630119294872 15.5637804660935046
  5.3548731279103761  2.6776387074344701  8.0909612769725197
  6.6941783072290368  4.0159262901463304  9.9214947331544341
  5.3552955253805727  2.6770855661686190 11.8277871014582328
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  6.6942371248290460  4.0156788297494526 13.7341181476547760
  5.3547750695152034  2.6773717025023229 15.5642088718491785
  5.3549639099020068  5.3549854485767199  8.0909423341568694
  6.6937401069779456  6.6937461220132013  9.9198655657292267
  5.3550306678636685  5.3550292648649016 11.8275277490694979
  6.6932850409585880  6.6932850628581511 13.7353432442495436
  5.3548001485768433  5.3548013106047883 15.5641142017244736

Interface: 3O-g-Al2O3(110)/fcc(100)_3x3/Os E_tot= -1179.85041749 eV
 D3-zero damping= -33.6391059 eV, D3-BJ damping= -42.2907516 eV
 O Al  O Al  O Al  O Os
 1.0000000000000000
     8.1252428492400028    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1252428492400028    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.5953160212026916
  18  12  24  16  12   8   3  45
Selective dynamics
Cartesian
  3.2991912187556491  7.2937851792404542 10.9423958550990683   F   F   F
  7.4580655726235303  4.9860759177604841  9.3854545373318246   F   F   F
  3.3001893815290155  6.9406864361766143  8.0000187449185951   F   F   F
  3.3958161689947715  3.1340947240615882  8.1990827428381010   F   F   F
  7.3627977056619249  1.1795248166082488  9.5845317789161761   F   F   F
  3.3890000976188133  2.9482450895698054 10.8220669229527680   F   F   F
  0.6618814033949375  3.1341734237544863  8.1993257849376420   F   F   F
  4.8200971285871885  1.1794232564928941  9.5846030099037201   F   F   F
  0.6690703814507163  2.9481214281409560 10.8217845066302907   F   F   F
  0.7585343175343413  7.2938904994894243 10.9423584978630899   F   F   F
  4.7240141799275719  4.9861628008527772  9.3853700880230981   F   F   F
  0.7574411950172799  6.9404356788656125  7.9999999999999991   F   F   F
  6.0911850042196027  7.1185373383441490 10.9172067463060039   F   F   F
  6.0911425489618907  7.2238124231900196  8.0327436308783255   F   F   F
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Oxide reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Os E_tot= -710.72714525 eV
 D3-zero damping= -11.407728 eV, D3-BJ damping= -17.0403887 eV
 O Al  O Al  O Al  H  O  H  O  H  O  H
 1.0000000000000000
     8.1252428492400028    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1252428492400028    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.2904852797336304
  18  12  24  16  12   8   1   1   1   1   1   1   3
Selective dynamics
Cartesian
  3.2991912187556491  7.2937851792404542 10.9423958550990683   F   F   F
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  1.7734147165579361  1.9506379355176953 19.3370056286922285   T   T   T
  6.1491976531090957  4.0237471111735168 17.8658648246861951   T   T   T
  7.6220198430981654  2.9173590112271626 19.4688936965206416   T   T   T
  1.7743948484578878  0.8758651794636902 20.6949674929612719   T   T   T
  1.2985379300146802  0.0332713476497997 20.5372574291625511   T   T   T
  4.6194098106537895  0.6483805252697873 20.5865148774531050   T   T   T
  3.8637374940625406  0.7922532971004181 21.1910459653911474   T   T   T
  2.1382892099134954  5.0242599754909616 20.4334157101558240   T   T   T
  2.0644226572787394  4.3036817539129641 21.0819317598477873   T   T   T
  3.6293168947628143  7.4636005824642462 19.8340589334067126   T   T   T
  5.9104993559063788  7.6196480725289240 19.8397227982018975   T   T   T

Metal reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Os E_tot= -488.15993705 eV
 D3-zero damping= -19.0922672 eV, D3-BJ damping= -21.8257468 eV
Os
 1.0000000000000000
     8.1252428492400028    0.0000000000000000    0.0000000000000000
     0.0000000000000000    8.1252428492400028    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0003327350601025 -0.0003346110310579  8.0726608277313492
  1.3538741175768974  1.3538740377712515  9.8838688012508111
 -0.0006213215287964 -0.0006210867386008 11.8277583989553854
  1.3535311440795212  1.3535335993101891 13.7715187921730688
 -0.0005808773649082 -0.0005834559026537 15.5827451483542401
 -0.0003323445937836  2.7076544285264514  8.0732543411712410
  1.3543135741350174  4.0623965012208352  9.8837887839751914
 -0.0005423914076921  2.7069404646696054 11.8277878366031324
  1.3541164706629185  4.0621066987414727 13.7715053263847196
 -0.0006586889950677  2.7073242333342296 15.5822488874604392
 -0.0002858251922651  5.4170370500658542  8.0731254457831980
  1.3539231961714231  6.7706584245364247  9.8838735619162410
 -0.0005854772143716  5.4170201526163160 11.8277866499189699
  1.3535388553480701  6.7702221242674741 13.7715310128444095
 -0.0006372923742848  5.4166299816664107 15.5823986643507642
  2.7076516850455947 -0.0003376291575535  8.0732515812766596
  4.0623958434547927  1.3543131476028316  9.8837901606286280
  2.7069405945475418 -0.0005428192943669 11.8277862506751053
  4.0621072620845462  1.3541172696110015 13.7715052064373129
  2.7073242787840943 -0.0006511975470205 15.5822455137109426
  2.7078991734544395  2.7078980565888213  8.0727266992488467
  4.0622935495383343  4.0622923645163285  9.8839738267261730
  2.7078347901388775  2.7078340720111571 11.8274777234662594
  4.0619818682628734  4.0619814396579681 13.7711806560253187
  2.7076553141432975  2.7076530587817005 15.5827338662937347
  2.7079594460400527  5.4166936362165821  8.0727080847598991
  4.0624567149622823  6.7703925099470226  9.8837740266492986
  2.7079024773733575  5.4165755562285760 11.8276483467345610
  4.0620622375568081  6.7701782285959959 13.7717319605329021
  2.7077365319745326  5.4162004974683100 15.5827929677851991
  5.4170413067926946 -0.0002732559020941  8.0731269910536980
  6.7706604413520886  1.3539216229925839  9.8838737606823859
  5.4170202257646487 -0.0005850191989876 11.8277870458024292
  6.7702225494835302  1.3535374565553151 13.7715324055711577
  5.4166239759709134 -0.0006470149525163 15.5824011821692974
  5.4166921840754938  2.7079567599721308  8.0727073119501362
  6.7703916888686306  4.0624572106795451  9.8837762768263548
  5.4165744015979689  2.7079035335379755 11.8276495651922033
  6.7701777117316402  4.0620635705562993 13.7717321305535734
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  5.4162010443114701  2.7077400368276767 15.5827914657268316
  5.4166622873822519  5.4166588459954994  8.0726629005991715
  6.7706673226347904  6.7706674785178897  9.8838693572360121
  5.4163504590435467  5.4163489836779357 11.8277907793031254
  6.7702378199766589  6.7702388689936583 13.7716573034948766
  5.4162006871495878  5.4162004123205847 15.5828540873254884

Interface: 3O-g-Al2O3(110)/fcc(100)_3x3/Ru E_tot= -1096.38909645 eV
 D3-zero damping= -33.7922648 eV, D3-BJ damping= -42.4287865 eV
 O Al  O Al  O Al  O Ru
 1.0000000000000000
     7.9985842258200019    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.9985842258200019    0.0000000000000000
     0.0000000000000000    0.0000000000000000   37.3375309279805094
  18  12  24  16  12   8   3  45
Selective dynamics
Cartesian
  3.2477624767573676  7.1800875572167371 10.9423958550990701   F   F   F
  7.3418071005591603  4.9083515317047208  9.3854545373318263   F   F   F
  3.2487450798822204  6.8324930189573090  8.0000187449185969   F   F   F
  3.3428812094701477  3.0852395537260136  8.1990827428381028   F   F   F
  7.2480242965192909  1.1611380443808434  9.5845317789161779   F   F   F
  3.3361713889759947  2.9022869968114313 10.8220669229527697   F   F   F
  0.6515638056348727  3.0853170266254546  8.1993257849376437   F   F   F
  4.7449600676543389  1.1610380674137890  9.5846030099037218   F   F   F
  0.6586407198322246  2.9021652630525163 10.8217845066302925   F   F   F
  0.7467100663386105  7.1801912357033624 10.9423584978630917   F   F   F
  4.6503748876444915  4.9084370604383718  9.3853700880230999   F   F   F
  0.7456339837298706  6.8322461705234216  8.0000000000000018   F   F   F
  5.9962338597497276  7.0075715300885992 10.9172067463060056   F   F   F
  5.9961920662967882  7.1112055566209627  8.0327436308783273   F   F   F
  1.9975346366254598  0.8823021113389700  9.5519775531218283   F   F   F
  1.9974259080813512  5.1185328113417841  9.4220834377914802   F   F   F
  5.9963226372818808  2.8749679828636467  8.1626394660302299   F   F   F
  5.9964022582387670  2.9745929312139707 10.8301543211852671   F   F   F
  0.6005743976438872  4.9029420940145254  8.0560139425344577   F   F   F
  4.5998937477725370  3.0907835395050367  9.5285274732362613   F   F   F
  0.6280548697736621  1.0952562825039629 10.9191009939757411   F   F   F
  7.3928886917428587  3.0907315817462386  9.5284873332419142   F   F   F
  3.3662962021694955  1.0953152275961158 10.9192047381793689   F   F   F
  3.3935879511956646  4.9028673068950512  8.0559839586400113   F   F   F
  5.9960819108915793  1.0030756487656995  8.1168144920444956   F   F   F
  5.9964365632120771  1.0022777150015598 10.8835529458276756   F   F   F
  5.9961472291028919  5.9621184458191046  9.4463612987341516   F   F   F
  1.9976025980708296  6.9904647313829278  9.4677862360962433   F   F   F
  1.9972708036911981  2.0315167946138590  8.1383270166926547   F   F   F
  1.9973780762061333  3.9882395811245073 10.8469192662674683   F   F   F
  3.2638691185406690  7.1182901029364007 16.5265798099969672   T   T   T
  7.3545372142241217  4.9089802483290095 14.9796374297886405   T   T   T
  3.2487450798822204  6.8324930189573090 13.5580397357678475   F   F   F
  7.3349405942879429  5.0911710234256331 12.3205669558782294   F   F   F
  7.2467807102846322  0.8135722636936886 12.2001224306209917   F   F   F
  3.3428812094701477  3.0852395537260136 13.7571037336873534   F   F   F
  7.2578794397790256  1.1434963999875702 15.1052393076694731   T   T   T
  3.3420127950498815  2.8701981305719575 16.4060560773955970   T   T   T
  4.7456874167695702  0.8134954666013710 12.2001609218852405   F   F   F
  0.6515638056348727  3.0853170266254546 13.7573467757868908   F   F   F
  4.7456022902981916  1.1394844284300285 15.1451271971230952   T   T   T
  0.6647155435969857  2.8701572351139975 16.4250058174889944   T   T   T
  0.7465597628193571  7.0968766946789135 16.5104649163995951   T   T   T
  4.6397390809007506  4.9120786897106532 14.9827339388584999   T   T   T
  0.7456339837298706  6.8322461705234216 13.5580209908492524   F   F   F
  4.6574979391432185  5.0910867014896573 12.3204488991888130   F   F   F
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5.9674356683447947	7.0176538263410668	16.5591441572455089	T	T	T
5.9961920662967882	7.1112055566209627	13.5907646217275779	F	F	F
1.9972155735817569	0.9859963745027107	12.2256103096605901	F	F	F
1.9930409924275074	0.8503873996037670	15.0768370890707768	T	T	T
2.0009685130638561	5.0916803390580432	14.9653720077834773	T	T	T
1.9972966691250460	5.0188778527719968	12.3122395822918431	F	F	F
5.9963226372818808	2.8749679828636467	13.7206604568794805	F	F	F
6.0033428730266607	2.9647872963538822	16.4436790453123400	T	T	T
0.6005743976438872	4.9029420940145254	13.6140349333837083	F	F	F
4.6271908518122293	6.8981473694906974	12.2234202596149490	F	F	F
4.6114332771186621	3.0937518442111385	15.1085205320804103	T	T	T
0.6114502544000890	1.0116270164749919	16.4061773868719349	T	T	T
7.3931691192467603	3.0905170760072065	15.1105386857244355	T	T	T
3.3430950105311990	1.0295323443879898	16.3860612505047740	T	T	T
3.3935879511956646	4.9028673068950512	13.6140049494892619	F	F	F
7.3653826576617032	6.8982048484045455	12.2233730105456448	F	F	F
5.9960819108915793	1.0030756487656995	13.6748354828937462	F	F	F
6.0262268323625818	1.0096392628539943	16.5164510967710250	T	T	T
5.9986518570254264	6.0111036953094912	15.0651077390903279	T	T	T
1.9938674456211682	6.9400234897053918	15.0756078059962988	T	T	T
1.9971483168511726	6.9914927226382924	12.2590327337071887	F	F	F
1.9972708036911981	2.0315167946138590	13.6963480075419053	F	F	F
2.0023917698506439	3.9962284700715216	16.3855901267134598	T	T	T
5.9962170088346873	4.0051593062072932	12.2955930440659973	F	F	F
3.3237300680070163	6.7675434703247328	19.1427326968052292	T	T	T
7.3093269136788530	5.0981122081819414	17.9684422008756215	T	T	T
7.3555689658650927	0.8556056527633117	17.7090340844831182	T	T	T
3.1699711845021326	2.8727184987840770	19.3733819911908611	T	T	T
4.6290962672431792	0.8671498052984017	17.7274770954054652	T	T	T
0.4027683156144012	3.1424962817378175	19.5945315631607393	T	T	T
0.6557825284930220	6.8143631787849115	19.1691269019382844	T	T	T
4.6550815260843255	4.9745392018050847	18.0221534698742225	T	T	T
5.9915643958329285	7.0943555929751616	19.2114409340205086	T	T	T
1.9881303977279678	0.9414010706398812	17.7400072507308835	T	T	T
1.9714763565455220	4.9370162661971611	17.8868509873618180	T	T	T
5.8492634809714330	2.9466115729692519	19.4450899562603645	T	T	T
0.5839665593655458	4.9179603664086304	19.1575688532012833	T	T	T
4.6652819581260356	6.8348863927089765	17.9260939499804799	T	T	T
3.3203570933967517	4.8305365377219864	19.1709272485802238	T	T	T
7.3239346099897418	6.9969115002231659	17.9396590932454814	T	T	T
4.5945571489619326	1.7911487947391256	19.1989996022896037	T	T	T
1.9927359120080961	7.0078195924508551	17.9396419934561280	T	T	T
1.5910111199208004	1.9985006679723312	19.0792357803922776	T	T	T
6.0560929634101059	3.9271010894579246	17.9761568459585277	T	T	T
1.7159636320909497	0.9757492736234278	20.5344149188508283	T	T	T
4.7182892660158702	0.8401500726650195	20.6886633314380184	T	T	T
1.9338168609967974	4.9802553112908283	20.4068146074745655	T	T	T
0.4755018258994019	-0.2625656855488035	21.5726621148501820	T	T	T
1.7757764964368303	1.1194559775130253	23.4952238211366051	T	T	T
0.4665452442820860	-0.1987277878084140	25.4060176140778040	T	T	T
0.4370942467726218	2.5180180958144911	21.6832864368601861	T	T	T
1.8015672944031793	3.7679319753277052	23.5779875293617884	T	T	T
0.4660728193459496	2.4534243521534180	25.4183627074260201	T	T	T
0.4695734284306871	5.1314564137130034	21.8694637991786749	T	T	T
1.8340950015302229	6.5158771058730940	23.5931569888414963	T	T	T
0.4691805115061314	5.1312888230882034	25.4738355666626468	T	T	T
3.1309252071528744	-0.2020419161392042	21.6629656071477719	T	T	T
4.4371916152287305	1.1775185761933931	23.5777624636722614	T	T	T
3.1579669122841114	-0.2124539093027230	25.4219385889737524	T	T	T
3.1365759135648852	2.5395570121920210	21.7964052710340042	T	T	T
4.5049219609439932	3.7829554786186983	23.5658531100560502	T	T	T
3.1598087049200125	2.4429349634116737	25.4191174379673193	T	T	T
3.2249542129420026	5.1410063619612485	21.8876588795301359	T	T	T

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  4.5310468987306747  6.5113444310975561 23.5147045637045800   T   T   T
  3.1686677657412323  5.1530204812953064 25.4244470772566551   T   T   T
  6.1047971518582145 -0.5899444166010664 21.1947725527609308   T   T   T
  7.0986290657557873  1.0712447613491221 23.3985092584006473   T   T   T
  5.8263856824829015 -0.1797658325931716 25.4598044562887793   T   T   T
  5.8023432571153615  2.5165466463381914 21.6509498103257094   T   T   T
  7.1368459772297692  3.7645750078805635 23.5168134188870646   T   T   T
  5.8263085548842204  2.4343962796843468 25.4545149329271965   T   T   T
  5.7899080358372386  5.0827421809076148 21.7485098850057419   T   T   T
  7.1390290398829608  6.4549862208429509 23.5479488712319629   T   T   T
  5.8325818711153534  5.1396301470101804 25.4775240467595872   T   T   T
  1.8091869070991922  1.1353575939466212 27.3376012987702985   T   T   T
  0.4881437337821909 -0.1884238711777744 29.1565683058691043   T   T   T
  1.8024625447352016  3.7923271422751546 27.3380664857994766   T   T   T
  0.4913827751230341  2.4529368582443420 29.1503499134206763   T   T   T
  1.8109669444350618  6.4649940685209453 27.3343027563671264   T   T   T
  0.4950639546844783  5.1296507187250855 29.1415225353515339   T   T   T
  4.4925207235328584  1.1317677554869583 27.3766106302542660   T   T   T
  3.1358442545190659 -0.2061740108366955 29.1484015326201167   T   T   T
  4.4786455499386486  3.7939367323264834 27.3360600088164922   T   T   T
  3.1417482018423990  2.4617995158652115 29.1464638056225454   T   T   T
  4.4797688260113766  6.4565842208463140 27.3563312578430313   T   T   T
  3.1520150222541767  5.1288563555127995 29.1364276275383283   T   T   T
  7.1442771536128866  1.1311789128597576 27.3652280921163715   T   T   T
  5.8209325687603739 -0.1948082868024604 29.1584854625785788   T   T   T
  7.1510960517810895  3.8192925199854257 27.3533581158670032   T   T   T
  5.8082848863611298  2.4680261182889325 29.1533396056315190   T   T   T
  7.1431605282876358  6.4659153926531463 27.3788547316574693   T   T   T
  5.8086544375324971  5.1189305728214327 29.1574687590164032   T   T   T

Oxide reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Ru E_tot= -709.37263716 eV
 D3-zero damping= -11.7329816 eV, D3-BJ damping= -17.5227515 eV
 O Al  O Al  O Al  H  O  H  O  H  O  H
 1.0000000000000000
     7.9985842258200019    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.9985842258200019    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.2904852797336304
  18  12  24  16  12   8   1   1   1   1   1   1   3
Selective dynamics
Cartesian
  3.2477624767573676  7.1800875572167371 10.9423958550990683   F   F   F
  7.3418071005591603  4.9083515317047208  9.3854545373318246   F   F   F
  3.2487450798822204  6.8324930189573090  8.0000187449185951   F   F   F
  3.3428812094701477  3.0852395537260136  8.1990827428381010   F   F   F
  7.2480242965192909  1.1611380443808434  9.5845317789161761   F   F   F
  3.3361713889759947  2.9022869968114313 10.8220669229527680   F   F   F
  0.6515638056348727  3.0853170266254546  8.1993257849376420   F   F   F
  4.7449600676543389  1.1610380674137890  9.5846030099037201   F   F   F
  0.6586407198322246  2.9021652630525163 10.8217845066302907   F   F   F
  0.7467100663386105  7.1801912357033624 10.9423584978630899   F   F   F
  4.6503748876444915  4.9084370604383718  9.3853700880230981   F   F   F
  0.7456339837298706  6.8322461705234216  8.0000000000000000   F   F   F
  5.9962338597497276  7.0075715300885992 10.9172067463060039   F   F   F
  5.9961920662967882  7.1112055566209627  8.0327436308783255   F   F   F
  1.9975346366254598  0.8823021113389700  9.5519775531218265   F   F   F
  1.9974259080813512  5.1185328113417841  9.4220834377914784   F   F   F
  5.9963226372818808  2.8749679828636467  8.1626394660302282   F   F   F
  5.9964022582387670  2.9745929312139707 10.8301543211852653   F   F   F
  0.6005743976438872  4.9029420940145254  8.0560139425344559   F   F   F
  4.5998937477725370  3.0907835395050367  9.5285274732362595   F   F   F
  0.6280548697736621  1.0952562825039629 10.9191009939757393   F   F   F
  7.3928886917428587  3.0907315817462386  9.5284873332419124   F   F   F
  3.3662962021694955  1.0953152275961158 10.9192047381793671   F   F   F
```

3.3935879511956646	4.9028673068950512	8.0559839586400095	F	F	F
5.9960819108915793	1.0030756487656995	8.1168144920444938	F	F	F
5.9964365632120771	1.0022777150015598	10.8835529458276739	F	F	F
5.9961472291028919	5.9621184458191046	9.4463612987341499	F	F	F
1.9976025980708296	6.9904647313829278	9.4677862360962415	F	F	F
1.9972708036911981	2.0315167946138590	8.1383270166926529	F	F	F
1.9973780762061333	3.9882395811245073	10.8469192662674665	F	F	F
3.2640619617665974	7.1308181638228874	16.5715297181337036	T	T	T
7.3607099966141067	4.9034212077405490	14.9786366830910893	T	T	T
3.2487450798822204	6.8324930189573090	13.5580397357678457	F	F	F
7.3349405942879429	5.0911710234256331	12.3205669558782276	F	F	F
7.2467807102846322	0.8135722636936886	12.2001224306209899	F	F	F
3.3428812094701477	3.0852395537260136	13.7571037336873516	F	F	F
7.2592686428172284	1.1366144512744694	15.1185269856226032	T	T	T
3.3399382567260396	2.8949634542727516	16.4193586538870591	T	T	T
4.7456874167695702	0.8134954666013710	12.2001609218852387	F	F	F
0.6515638056348727	3.0853170266254546	13.7573467757868890	F	F	F
4.7321575167517249	1.1336454028861671	15.1743826368724370	T	T	T
0.6462531543503990	2.8837006753562138	16.4190818091684072	T	T	T
0.7629341007818962	7.1084739148439242	16.5121718024434827	T	T	T
4.6381490102699106	4.9121849596541285	14.9830950287099753	T	T	T
0.7456339837298706	6.8322461705234216	13.5580209908492506	F	F	F
4.6574979391432185	5.0910867014896573	12.3204488991888113	F	F	F
5.9845952376913205	6.9852322698683649	16.5221564078856424	T	T	T
5.9961920662967882	7.1112055566209627	13.5907646217275762	F	F	F
1.9972155735817569	0.9859963745027107	12.2256103096605884	F	F	F
2.0036562953220733	0.8675104471889340	15.1198219272043541	T	T	T
2.0029411184012789	5.1052186316922201	14.9799366541941925	T	T	T
1.9972966691250460	5.0188778527719968	12.3122395822918413	F	F	F
5.9963226372818808	2.8749679828636467	13.7206604568794788	F	F	F
6.0010244084675168	2.9652275937400532	16.3942295913057379	T	T	T
0.6005743976438872	4.9029420940145254	13.6140349333837065	F	F	F
4.6271908518122293	6.8981473694906974	12.2234202596149473	F	F	F
4.6027380775412903	3.0851914104853742	15.1012289074143613	T	T	T
0.6148727533265098	1.0477981024524634	16.4622408403676062	T	T	T
7.3921356164466294	3.0762034461603660	15.0909610573147113	T	T	T
3.3436120551120481	1.0743948551889584	16.4716572497394722	T	T	T
3.3935879511956646	4.9028673068950512	13.6140049494892601	F	F	F
7.3653826576617032	6.8982048484045455	12.2233730105456431	F	F	F
5.9960819108915793	1.0030756487656995	13.6748354828937444	F	F	F
6.0190538938504385	1.0128062301565781	16.5297804546337055	T	T	T
6.0062574736228154	5.9981836802365205	15.0254522384564808	T	T	T
1.9903284404864989	6.9633933940939423	15.0638486769352173	T	T	T
1.9971483168511726	6.9914927226382924	12.2590327337071869	F	F	F
1.9972708036911981	2.0315167946138590	13.6963480075419035	F	F	F
1.9835701612830869	3.9981156847166601	16.3945914156157961	T	T	T
5.9962170088346873	4.0051593062072932	12.2955930440659955	F	F	F
3.3639272265890168	6.7290620161383865	19.1423727732584759	T	T	T
7.3672461938199891	5.0640795518962873	17.9840514381140864	T	T	T
7.3372559994506910	0.8099875186824461	17.7207750015915479	T	T	T
3.2727613058813043	2.8609092680273163	19.4364668482208351	T	T	T
4.6520144548384765	0.8697061537734715	17.8009332492537204	T	T	T
0.4685909600605732	3.1584069365364327	19.5916424093193164	T	T	T
0.6848341114542043	6.7791028183619968	19.1718593756880864	T	T	T
4.6455461807645531	4.9510538145577128	18.0057585375069245	T	T	T
5.9706083556752230	6.9139871813422138	19.1239416218351046	T	T	T
1.9754497748609927	0.9653363686489463	17.8523418599032766	T	T	T
2.0188399029430704	4.9521381816093903	17.9075521812137772	T	T	T
6.0406695165009143	2.9035607585544576	19.3056989588247845	T	T	T
0.6758032096115947	4.9457440821675211	19.1924601644613908	T	T	T
4.6746507348988828	6.7964492501319151	17.8012522135597138	T	T	T
3.3296152285844993	4.6634185644153909	19.1419164481702992	T	T	T
7.3548035595584658	6.9533676136118245	17.9081786876182676	T	T	T

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  4.7222905761066585  1.7933806734378508 19.3678134095372556   T   T   T
  1.9705409700238210  7.0398545614173926 17.9311943177312330   T   T   T
  1.7244790161796679  1.9031707754395992 19.3970945768573877   T   T   T
  6.0673088326590641  3.9375663022424048 17.8839685098164232   T   T   T
  7.4389471175369399  2.8713821786901641 19.5420386750259496   T   T   T
  1.7479656807892590  0.8338013573876731 20.7609086197490207   T   T   T
  1.2883037769276884 -0.0163575937537460 20.5870547963018673   T   T   T
  4.5321863802585165  0.6113330081881976 20.6594393732499206   T   T   T
  3.7254062840772839  0.7541106300474505 21.2033170005473437   T   T   T
  2.1102377390313647  4.9611269998614853 20.5225710797450347   T   T   T
  2.0340286874842661  4.2282567818347054 21.1572542760739140   T   T   T
  3.6167290067571916  7.3557509811339088 19.8882588576956039   T   T   T
  5.8419145627823994  7.4818151073305863 19.9055761366124031   T   T   T

Metal reference: 3O-g-Al2O3(110)/fcc(100)_3x3/Ru E_tot= -405.36638166 eV
 D3-zero damping= -18.3989542 eV, D3-BJ damping= -21.5203814 eV
Ru
 1.0000000000000000
     7.9985842258200019    0.0000000000000000    0.0000000000000000
     0.0000000000000000    7.9985842258200019    0.0000000000000000
     0.0000000000000000    0.0000000000000000   23.6545931140760395
  45
Cartesian
 -0.0038453081226937 -0.0004090309230234  8.1265508146813232
  1.3336832682896687  1.3332538190226704  9.9182356994329890
 -0.0000120299327283 -0.0003080689488928 11.8283961194142169
  1.3334964701589767  1.3332254513509585 13.7380356488609827
 -0.0018349130475245 -0.0043411702989405 15.5292313602483674
 -0.0007501370339095  2.6648461734405706  8.1209770823533773
  1.3327594926721886  3.9981485634376641  9.9174410603996694
 -0.0001741299985207  2.6665151789543224 11.8279891409823783
  1.3333301836930633  3.9988160419761281 13.7384648973183623
 -0.0001143182330345  2.6652580608646441 15.5343526279817148
 -0.0004826020321127  5.3336130020245731  8.1212219729904618
  1.3327846926936109  6.6638002002111998  9.9186428154775594
 -0.0000347841192725  5.3316258466738393 11.8275103737889271
  1.3341056398064759  6.6635775256955263 13.7357557688178780
 -0.0006038727371930  5.3330047555171065 15.5339359450231047
  2.6650699096514865 -0.0002253969042696  8.1202738013201863
  3.9984991651283228  1.3331158681288411  9.9166767775708085
  2.6668098524861081 -0.0000149974689690 11.8274764294360057
  3.9985892512010661  1.3331750770426378 13.7378705283150815
  2.6654303716887235 -0.0001553975964232 15.5344267610478646
  2.6636185907374448  2.6638848259855643  8.1201687730425434
  3.9991198765365974  3.9992760728780752  9.9185085779172972
  2.6660345851853267  2.6660897680477609 11.8277483464038493
  3.9990617586855839  3.9991701079187298 13.7361288066715659
  2.6633520957420957  2.6634720830853174 15.5352306371314377
  2.6634186163688018  5.3339441233049305  8.1200392423445376
  3.9980975690195106  6.6653542706119087  9.9176328052417873
  2.6663639032122366  5.3322103968300674 11.8272868278348113
  3.9989486692890752  6.6651058012433841 13.7387946478045073
  2.6640579638168123  5.3331283136935328 15.5351956676340457
  5.3336020350540041 -0.0000018789249453  8.1218611402136425
  6.6640486199010347  1.3342429738993893  9.9211930018591765
  5.3318321400964130 -0.0000166368529822 11.8280263699813144
  6.6640042984428112  1.3323335842284534 13.7373658420724158
  5.3329849746499178 -0.0005435519606291 15.5342149998015966
  5.3344214131441490  2.6641839059998689  8.1203505057087888
  6.6648616837131840  3.9989218086534581  9.9166519760450793
  5.3319792239929749  2.6664696242473140 11.8276671933943760
  6.6652072953531745  3.9977673965570308 13.7369358690993408
  5.3338521812397692  2.6639162017226563 15.5349001825971325
```

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  5.3336856462435618  5.3349534450696501  8.1203853179516745
  6.6638636481564761  6.6643572865489480  9.9211916001911753
  5.3311417325205239  5.3315720763010024 11.8278292993229819
  6.6639313427553564  6.6636053739618371 13.7337967586346199
  5.3349340364375015  5.3332103024600821 15.5348227253362090

Interface: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Ag E_tot= -626.05649029 eV
 D3-zero damping= -45.2435502 eV, D3-BJ damping= -48.7108856 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Ag
 1.0000000000000000
    12.2210412709508383    0.0000000000000000    0.0000000000000000
     0.0000000000000000   16.2947216946011189    0.0000000000000000
     0.0000000000000000    0.0000000000000000   27.0258439111562545
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2  72
Selective dynamics
Cartesian
  4.0738335747809264  0.0050797044791747  8.0000000000000000   F   F   F
  2.0369924110343360  2.7208666593272204  8.0000055199296671   F   F   F
  4.0738334579494468  2.0643499433894039  8.0000008619369254   F   F   F
  2.0369931855636443  4.7801369014372304  8.0000049280612373   F   F   F
  1.0185673986168704  0.0050797243494278  9.6370125635575068   F   F   F
  5.0922468703456980  2.7208666791974734  9.6370180834871757   F   F   F
  1.0185672817853899  2.0643499632596569  9.6370134254944340   F   F   F
  5.0922476448750071  4.7801369213074834  9.6370174916187459   F   F   F
  4.0308551292296029  0.0296392740443985 11.2774950239311309   T   T   T
  2.1036012454541844  2.7133551097809625 11.2663208570362787   T   T   T
  4.0169986919290563  2.0582748493220016 11.2650128768001832   T   T   T
  2.1013488754182039  4.7418183736721842 11.2302079759909681   T   T   T
  0.8591377502035711  0.0307640921498222 12.6211715230184005   T   T   T
  5.2058209378976423  2.7579948014855820 12.6812967690606673   T   T   T
  0.8653894962291643  1.9928725895154571 12.6304817167351082   T   T   T
  5.1523425100256830  4.7586242926434252 12.6862967469092744   T   T   T
  4.0738337492903769  5.4366536026795442  8.0000000000000000   F   F   F
  2.0369925855437869  8.1524405575275907  8.0000055199296671   F   F   F
  4.0738336324588982  7.4959238415897742  8.0000008619369254   F   F   F
  2.0369933600730956 10.2117107996376006  8.0000049280612373   F   F   F
  1.0185675731263213  5.4366536225497981  9.6370125635575068   F   F   F
  5.0922470448551493  8.1524405773978454  9.6370180834871757   F   F   F
  1.0185674562948410  7.4959238614600281  9.6370134254944340   F   F   F
  5.0922478193844585 10.2117108195078536  9.6370174916187459   F   F   F
  3.9882102369397692  5.4234877485998618 11.2134401549342666   T   T   T
  2.1012851152524252  8.1837340749790712 11.1896434222229821   T   T   T
  3.9711185335279526  7.4541357766794043 11.1999479273387479   T   T   T
  2.1305525812157442 10.2047555736951789 11.2237071714705507   T   T   T
  0.9881557458006976  5.4601292386638862 12.6750163352434804   T   T   T
  5.0898702839159693  8.2142631673525255 12.5921617444587266   T   T   T
  0.9581347014226719  7.4430390816377097 12.6348964311603424   T   T   T
  5.1756682508589842 10.1772648141722311 12.6193240529969835   T   T   T
  4.0738339237998291 10.8682275008799163  8.0000000000000000   F   F   F
  2.0369927600532378 13.5840144557279636  8.0000055199296671   F   F   F
  4.0738338069683495 12.9274977397901463  8.0000008619369254   F   F   F
  2.0369935345825465 15.6432846978379718  8.0000049280612373   F   F   F
  1.0185677476357724 10.8682275207501693  9.6370125635575068   F   F   F
  5.0922472193645998 13.5840144755982131  9.6370180834871757   F   F   F
  1.0185676308042919 12.9274977596603993  9.6370134254944340   F   F   F
  5.0922479938939080 15.6432847177082248  9.6370174916187459   F   F   F
  4.0145206974556604 10.9311275899549578 11.2108742943618562   T   T   T
  2.0944267418877889 13.6255570588361685 11.2593829672193149   T   T   T
  4.0124668477585876 12.9456546423650796 11.2611204421700890   T   T   T
  2.1148131149127782 15.6430536979696697 11.2586698382717554   T   T   T
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0.9197785629120661	10.9418367054937082	12.5701859425005331	T	T	T
5.2674626922333063	13.6721969217514410	12.6025666849036906	T	T	T
0.9028231765953361	12.9032958740965213	12.6663842124169701	T	T	T
5.2800861448469290	15.6224040533626614	12.6456773242013796	T	T	T
10.1843542102563447	0.0050797044791747	8.0000000000000000	F	F	F
8.1475130465097543	2.7208666593272204	8.0000055199296671	F	F	F
10.1843540934248651	2.0643499433894039	8.0000008619369254	F	F	F
8.1475138210390625	4.7801369014372304	8.0000049280612373	F	F	F
7.1290880340922875	0.0050797243494278	9.6370125635575068	F	F	F
11.2027675058211180	2.7208666791974734	9.6370180834871757	F	F	F
7.1290879172608088	2.0643499632596569	9.6370134254944340	F	F	F
11.2027682803504263	4.7801369213074834	9.6370174916187459	F	F	F
10.1202571021481340	0.0362941085552730	11.1897851278646190	T	T	T
8.2070627162172300	2.7837756715862620	11.2107743524695458	T	T	T
10.0910056964483790	2.0573187440868028	11.2237808536427810	T	T	T
8.2089377993793278	4.7983077588095835	11.2611053906667493	T	T	T
7.1315737987218615	0.0669218899421910	12.5920781965165745	T	T	T
11.3016964639516519	2.7944104022129221	12.5701713056323339	T	T	T
7.0458018384452945	2.0299933622751443	12.6193067187606403	T	T	T
11.3186713378307910	4.7559324910541294	12.6665397092309515	T	T	T
10.1843543847657969	5.4366536026795442	8.0000000000000000	F	F	F
8.1475132210192065	8.1524405575275907	8.0000055199296671	F	F	F
10.1843542679343138	7.4959238415897742	8.0000008619369254	F	F	F
8.1475139955485130	10.2117107996376006	8.0000049280612373	F	F	F
7.1290882086017389	5.4366536225497981	9.6370125635575068	F	F	F
11.2027676803305685	8.1524405773978454	9.6370180834871757	F	F	F
7.1290880917702601	7.4959238614600281	9.6370134254944340	F	F	F
11.2027684548598767	10.2117108195078536	9.6370174916187459	F	F	F
10.1270482227335403	5.4780344419136489	11.2594422766114270	T	T	T
8.1904452724624566	8.1770578689195617	11.2773047344596051	T	T	T
10.1065747015181522	7.4956817340408231	11.2586968467625113	T	T	T
8.2043656163211374	10.2056540381450525	11.2649429823292806	T	T	T
6.9540537347085749	5.5248780447756065	12.6027109195867695	T	T	T
11.3623631964334990	8.1781911852848772	12.6208650159728801	T	T	T
6.9413260736169589	7.4750885787715760	12.6456332083927112	T	T	T
11.3561183408255086	10.1402827580562498	12.6304147827127480	T	T	T
10.1843545592752474	10.8682275008799163	8.0000000000000000	F	F	F
8.1475133955286569	13.5840144557279636	8.0000055199296671	F	F	F
10.1843544424437660	12.9274977397901463	8.0000008619369254	F	F	F
8.1475141700579652	15.6432846978379718	8.0000049280612373	F	F	F
7.1290883831111902	10.8682275207501693	9.6370125635575068	F	F	F
11.2027678548400189	13.5840144755982131	9.6370180834871757	F	F	F
7.1290882662797097	12.9274977596603993	9.6370134254944340	F	F	F
11.2027686293693289	15.6432847177082248	9.6370174916187459	F	F	F
10.1177935069602913	10.8606891972500943	11.2663827557580980	T	T	T
8.2331924169208150	13.5709839763938245	11.2134715820854840	T	T	T
10.1201795470034099	12.8892351723978056	11.2303009763298807	T	T	T
8.2502811381731878	15.6015916254917304	11.1999820274967519	T	T	T
7.0156092501901473	10.9052839930790615	12.6813711173255061	T	T	T
11.2334028862195119	13.6074009835631298	12.6751795490835359	T	T	T
7.0691707800618380	12.9059977098784806	12.6862570106854609	T	T	T
11.2635012463775475	15.5904399771926325	12.6350347394720153	T	T	T
0.1108634922268933	2.0089720903926125	14.9391292386433001	T	T	T
2.1366767417426966	-0.0176979855069905	14.9554934025080382	T	T	T
-0.0085128701977628	0.0112112042898756	16.9179113561689185	T	T	T
2.0387332007182568	2.0519004169438175	16.9980234983457521	T	T	T
-0.0483658200232561	2.0379610538842163	18.9470912546970567	T	T	T
2.0162536207650565	0.0005854184676767	19.0342347363535183	T	T	T
-0.1098688641499837	6.1555039150932123	14.9635487132063361	T	T	T
2.0480713587014034	4.0877088910046648	14.7514393059729922	T	T	T
0.0080058167779832	4.0713840027582870	16.8908970837021926	T	T	T
2.0701062188630206	6.1400250752290937	16.7459886737830779	T	T	T
0.0500293417233539	6.1118928083783342	18.9284731145315668	T	T	T

2.0416452233777336	4.0962837050766741	18.9604083551934224	T	T	T
-0.1106819644895988	10.1562893858614682	14.9390101980149623	T	T	T
2.0625240435678673	8.2019458669414114	14.5533079224147457	T	T	T
0.0086248506818574	8.1585363553242374	16.9177969900252272	T	T	T
2.0542893918155802	10.1625189519570096	16.7360898008472674	T	T	T
0.0485135359514638	10.1852865208076864	18.9471185906787518	T	T	T
2.0869654016334613	8.1520342601431199	18.8415220973525877	T	T	T
0.1101089960654697	14.3028639991564042	14.9636120077130226	T	T	T
2.0354820774031430	12.2327348058797511	14.7423220979368885	T	T	T
-0.0078969078676611	12.2187709223642500	16.8908424745936792	T	T	T
2.0417674871329345	14.2463063101576601	16.9913934488634233	T	T	T
-0.0499262645971665	14.2592780556586511	18.9284401574414609	T	T	T
2.0397381270539805	12.1956586123791357	18.9422187673313118	T	T	T
3.9671753499862277	2.0587093030506249	14.9078378837970380	T	T	T
5.9018065447636747	0.0102396626074798	14.8955345123294283	T	T	T
4.0661197635753092	-0.0018634162574493	17.0260226793755969	T	T	T
6.1073971453540148	2.0178900499630954	16.8760916105898318	T	T	T
4.0925717636994250	2.0551929363119474	19.0023387477950578	T	T	T
6.1665820433891332	-0.0010982826374344	18.9331915981385102	T	T	T
4.0677813240499994	6.1075591745988849	14.5461334160214477	T	T	T
6.1261466146605938	4.0725811323879970	14.9517403846943271	T	T	T
4.0523949622897160	4.1061975416971332	16.8752507094012287	T	T	T
6.0994906025993272	6.1289872274595742	16.8722189155136242	T	T	T
4.0588934519282436	6.1282375852617905	18.8774591680894090	T	T	T
6.1118686801382580	4.0729549450335147	18.9019775405658308	T	T	T
4.0459408088416220	10.2535706438310843	14.6500575391646137	T	T	T
6.3194226490745891	8.1576777094352853	14.8956111421395097	T	T	T
4.0766209564706974	8.1367808987891674	16.6498457594652223	T	T	T
6.1137960216413365	10.1652542315950871	16.8761200240766414	T	T	T
4.0573368750727168	10.1659078586671558	18.8607793937322725	T	T	T
6.0546733857784494	8.1462542382795942	18.9331441461375967	T	T	T
3.9801812538731181	14.2162761482052886	14.8931238925883918	T	T	T
6.0950221022987892	12.2200666109878977	14.9517173180078782	T	T	T
4.0441993751873921	12.1959957777346979	16.8666954553563535	T	T	T
6.1215793990122398	14.2762443355665152	16.8722598649942412	T	T	T
4.0964846378247657	14.2377038408498713	18.9942335027058711	T	T	T
6.1092180040233002	12.2202394395965417	18.9020970952341010	T	T	T
8.1750841293298251	2.1059078721552402	14.6501746415028649	T	T	T
10.1586659546019060	0.0546206938299174	14.5533135283206096	T	T	T
8.1445539575408503	-0.0107004754056997	16.6498707481988149	T	T	T
10.1668328278658109	2.0151746935272410	16.7360954743286925	T	T	T
8.1637057274413394	2.0186272959953042	18.8607643358998622	T	T	T
10.1340427411270060	0.0046714891866596	18.8414962357120110	T	T	T
8.2410553059426164	6.0689397035986481	14.8931191638433109	T	T	T
10.1857506759180758	4.0853188643416702	14.7422850709909579	T	T	T
8.1770388731826635	4.0487067432659520	16.8666650839510055	T	T	T
10.1794514190971164	6.0989744369167989	16.9913538524616392	T	T	T
8.1246449122175282	6.0905454871306759	18.9942606316426996	T	T	T
10.1814113508813691	4.0483353018685211	18.9422362825790671	T	T	T
8.2540220217859908	10.2062348065085668	14.9076677952758754	T	T	T
10.0844913902641213	8.1296782118147632	14.9552316498774065	T	T	T
8.1550679346248511	8.1454679899929872	17.0259305292491234	T	T	T
10.1824749641984305	10.1992185035127747	16.9979254712467025	T	T	T
8.1286546191554852	10.2025174283567850	19.0022162769472907	T	T	T
10.2049530133646229	8.1479760173018256	19.0342904412556990	T	T	T
8.1534488229093700	14.2549381617019204	14.5460290442625606	T	T	T
10.1730347628657327	12.2351630496612671	14.7513038041444684	T	T	T
8.1687936905060834	12.2535468184021514	16.8752589618359004	T	T	T
10.1510779280577754	14.2873470192714453	16.7459841865539261	T	T	T
8.1621990169965493	14.2755041784032599	18.8774421387278579	T	T	T
10.1794626389598104	12.2435962740689810	18.9603746183728390	T	T	T

```
Oxide reference: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Ag E_tot= -413.2187021
eV
 D3-zero damping= -12.1555499 eV, D3-BJ damping= -13.2367012 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
    12.2210412709508383    0.0000000000000000    0.0000000000000000
     0.0000000000000000   16.2947216946011189    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.6962294882237074
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  4.0738335747809264  0.0050797044791747  8.0000000000000000   F   F   F
  2.0369924110343360  2.7208666593272204  8.0000055199296689   F   F   F
  4.0738334579494468  2.0643499433894039  8.0000008619369254   F   F   F
  2.0369931855636443  4.7801369014372304  8.0000049280612373   F   F   F
  1.0185673986168704  0.0050797243494278  9.6370125635575086   F   F   F
  5.0922468703456980  2.7208666791974734  9.6370180834871775   F   F   F
  1.0185672817853899  2.0643499632596569  9.6370134254944340   F   F   F
  5.0922476448750071  4.7801369213074834  9.6370174916187459   F   F   F
  3.9878388479433489  0.0260078274352656 11.2677563495351301   T   T   T
  2.1245614593048909  2.7493706860197533 11.2678283811530555   T   T   T
  4.0290628504939434  2.0637311012608031 11.2661054834404926   T   T   T
  2.0813765501144577  4.7841953809679509 11.2672866823776889   T   T   T
  0.7321122033868961  0.1796972812475199 12.4804582725340527   T   T   T
  5.3763507846338054  2.8887868252236171 12.4787415716480137   T   T   T
  0.9579628970387416  2.0461111624405790 12.7038233558930376   T   T   T
  5.1511198573963473  4.7571653742353028 12.7031710260902457   T   T   T
  4.0738337492903769  5.4366536026795442  8.0000000000000000   F   F   F
  2.0369925855437869  8.1524405575275907  8.0000055199296689   F   F   F
  4.0738336324588982  7.4959238415897742  8.0000008619369254   F   F   F
  2.0369933600730956 10.2117107996376006  8.0000049280612373   F   F   F
  1.0185675731263213  5.4366536225497981  9.6370125635575086   F   F   F
  5.0922470448551493  8.1524405773978454  9.6370180834871775   F   F   F
  1.0185674562948410  7.4959238614600281  9.6370134254944340   F   F   F
  5.0922478193844585 10.2117108195078536  9.6370174916187459   F   F   F
  3.9886111692153450  5.4657039264035792 11.2674183911949548   T   T   T
  2.1230172945389412  8.1733458170894888 11.2676162286047195   T   T   T
  4.0304082366510920  7.4979464404006322 11.2675294608372685   T   T   T
  2.0818647314646674 10.2110672852618976 11.2660639592292053   T   T   T
  0.7285675680029726  5.6059660166273586 12.4776043106820698   T   T   T
  5.3786072990879825  8.3270301696424731 12.4804493351806034   T   T   T
  0.9548294471538042  7.4729603146940438 12.7027994765770771   T   T   T
  5.1530077343806768 10.1935721528506509 12.7038586120503076   T   T   T
  4.0738339237998291 10.8682275008799163  8.0000000000000000   F   F   F
  2.0369927600532378 13.5840144557279636  8.0000055199296689   F   F   F
  4.0738338069683495 12.9274977397901463  8.0000008619369254   F   F   F
  2.0369935345825465 15.6432846978379718  8.0000049280612373   F   F   F
  1.0185677476357724 10.8682275207501693  9.6370125635575086   F   F   F
  5.0922472193645998 13.5840144755982131  9.6370180834871775   F   F   F
  1.0185676308042919 12.9274977596603993  9.6370134254944340   F   F   F
  5.0922479938939080 15.6432847177082248  9.6370174916187459   F   F   F
  3.9863647440707566 10.8968014160082518 11.2679413378404245   T   T   T
  2.1222895229030976 13.6131284950851370 11.2673180809747215   T   T   T
  4.0295017505152897 12.9315644782369379 11.2672752094716628   T   T   T
  2.0804466285107459 15.6453216822351884 11.2675250040883164   T   T   T
  0.7346133341236757 11.0361131424289898 12.4788073354065912   T   T   T
  5.3823123830810307 13.7532880551048287 12.4776293216717207   T   T   T
  0.9597847101675572 12.9045611194974477 12.7031279192265281   T   T   T
  5.1559516434645714 15.6202789117433731 12.7028594223074869   T   T   T
 10.1843542102563447  0.0050797044791747  8.0000000000000000   F   F   F
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  8.1475130465097543  2.7208666593272204  8.0000055199296689   F   F   F
 10.1843540934248651  2.0643499433894039  8.0000008619369254   F   F   F
  8.1475138210390625  4.7801369014372304  8.0000049280612373   F   F   F
  7.1290880340922875  0.0050797243494278  9.6370125635575086   F   F   F
 11.2027675058211180  2.7208666791974734  9.6370180834871775   F   F   F
  7.1290879172608088  2.0643499632596569  9.6370134254944340   F   F   F
 11.2027682803504263  4.7801369213074834  9.6370174916187459   F   F   F
 10.0983595448707018  0.0260078344303952 11.2677564518752806   T   T   T
  8.2350821258484554  2.7493706829224278 11.2678283848530576   T   T   T
 10.1395833437041993  2.0637311293388403 11.2661054778610907   T   T   T
  8.1918970866889254  4.7841953527511318 11.2672866836747705   T   T   T
  6.8426329109243849  0.1796972860168201 12.4804582894798823   T   T   T
 11.4868713602882444  2.8887868830511358 12.4787415921604925   T   T   T
  7.0684835566598609  2.0461111314156342 12.7038234319443433   T   T   T
 11.2616405606683134  4.7571654902379263 12.7031710626639018   T   T   T
 10.1843543847657969  5.4366536026795442  8.0000000000000000   F   F   F
  8.1475132210192065  8.1524405575275907  8.0000055199296689   F   F   F
 10.1843542679343138  7.4959238415897742  8.0000008619369254   F   F   F
  8.1475139955485130 10.2117107996376006  8.0000049280612373   F   F   F
  7.1290882086017389  5.4366536225497981  9.6370125635575086   F   F   F
 11.2027676803305685  8.1524405773978454  9.6370180834871775   F   F   F
  7.1290880917702601  7.4959238614600281  9.6370134254944340   F   F   F
 11.2027684548598767 10.2117108195078536  9.6370174916187459   F   F   F
 10.0991317692078937  5.4657038533495497 11.2674185094975101   T   T   T
  8.2335378918791076  8.1733459501179961 11.2676162557297133   T   T   T
 10.1409288184327533  7.4979463584474377 11.2675294845757286   T   T   T
  8.1923852624925928 10.2110673923077417 11.2660640314155795   T   T   T
  6.8390880352783165  5.6059660284275550 12.4776042183341076   T   T   T
 11.4891278942790169  8.3270300886524069 12.4804491632130663   T   T   T
  7.0653500349673433  7.4729602654960994 12.7027994185201205   T   T   T
 11.2635284078764162 10.1935721186804145 12.7038585668221486   T   T   T
 10.1843545592752474 10.8682275008799163  8.0000000000000000   F   F   F
  8.1475133955286569 13.5840144557279636  8.0000055199296689   F   F   F
 10.1843544424437660 12.9274977397901463  8.0000008619369254   F   F   F
  8.1475141700579652 15.6432846978379718  8.0000049280612373   F   F   F
  7.1290883831111902 10.8682275207501693  9.6370125635575086   F   F   F
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  7.1290882662797097 12.9274977596603993  9.6370134254944340   F   F   F
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 10.0968853569315051 10.8968014481868813 11.2679414344617950   T   T   T
  8.2328102227761182 13.6131284888837438 11.2673180858552850   T   T   T
 10.1400223610236822 12.9315643468487256 11.2672751199290477   T   T   T
  8.1909671749404644 15.6453217289422213 11.2675250040883164   T   T   T
  6.8451338829370094 11.0361132059142797 12.4788075254219564   T   T   T
 11.4928331153186800 13.7532879499338385 12.4776292259917057   T   T   T
  7.0703052858378870 12.9045611692632569 12.7031279067645819   T   T   T
 11.2664723132309774 15.6202788360051272 12.7028594171937499   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Ag E_tot= -196.52705736
eV
 D3-zero damping= -21.5752725 eV, D3-BJ damping= -27.1643957 eV
Ag
 1.0000000000000000
    12.2210412709508383    0.0000000000000000    0.0000000000000000
     0.0000000000000000   16.2947216946011189    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.1082705496269156
  72
Cartesian
 -0.0000000084546683  2.0368402260854372  7.9932978100821064
  2.0368402118251407  0.0000000142857475  7.9932977143556316
 -0.0000000000000000  0.0000000370007108 10.0541353731665009
  2.0368402118251407  2.0368402488004000 10.0541353874522397
  0.0000000000000000  2.0368402403711872 12.1149730377933746
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2.0368402033704744	0.0000000000000000	12.1149730748345732
0.0000000000000000	6.1105206354754200	7.9932977683362330
2.0368402118251407	4.0736804236502797	7.9932977455807785
-0.0000000000000000	4.0736804320795041	10.0541353731665311
2.0368402118251407	6.1105206211896812	10.0541354017379785
0.0000000142857475	6.1105206211896812	12.1149730436094050
2.0368402033704744	4.0736804236502797	12.1149730150379220
0.0000000227149633	10.1842010448399609	7.9932977085396173
2.0368401891101771	8.1473608330402705	7.9932977312950699
0.0000000000000000	8.1473608245855971	10.0541353731665009
2.0368402118251407	10.1842010221504484	10.0541353874522397
0.0000000142857475	10.1842010448654108	12.1149730520791135
2.0368402118251407	8.1473608473005594	12.1149730293236608
0.0000000000000000	14.2578814970617174	7.9932976630287103
2.0368402261108907	12.2210412709508400	7.9932977000698715
-0.0000000000000000	12.2210412482613258	10.0541353874522397
2.0368402118251407	14.2578814970617174	10.0541353874522397
0.0000000000000000	14.2578814827759786	12.1149730975900205
2.0368402118251407	12.2210412709508400	12.1149730891203120
4.0736804236502815	2.0368402118251399	7.9932977371110843
6.1105206581903824	-0.0000000000000000	7.9932977143556316
4.0736804236502815	0.0000000369752582	10.0541353874522397
6.1105206354754191	2.0368402345401031	10.0541353731665311
4.0736804321049549	2.0368402118251399	12.1149730377933746
6.1105206355008690	-0.0000000000000000	12.1149730748345732
4.0736804236502815	6.1105206211896812	7.9932977455807785
6.1105206354754191	4.0736804236502797	7.9932978328375608
4.0736804236502815	4.0736804236502797	10.0541353874522397
6.1105206354754191	6.1105206211896812	10.0541353874522397
4.0736804093645427	6.1105206354754200	12.1149730293236608
6.1105206354754191	4.0736804379105687	12.1149730150379220
4.0736804236502815	10.1842010591256997	7.9932977228253241
6.1105206497357081	8.1473608473005594	7.9932977455807785
4.0736804379105704	8.1473608245855971	10.0541354017379483
6.1105206354754191	10.1842010221504484	10.0541353874522397
4.0736804379105704	10.1842010448654108	12.1149730663648967
6.1105206439300934	8.1473608472751096	12.1149730293236608
4.0736804236502815	14.2578814827759786	7.9932976857841629
6.1105206354754191	12.2210412566905511	7.9932976857841629
4.0736804236502815	12.2210412709508400	10.0541353731665311
6.1105206354754191	14.2578814970617174	10.0541354017379483
4.0736804236502815	14.2578814970617174	12.1149730891203120
6.1105206354754191	12.2210412709508400	12.1149731034060952
8.1473608330402669	2.0368402261108898	7.9932977228253241
10.1842010818661137	0.0000000142857475	7.9932977143556316
8.1473608473005577	0.0000000227149633	10.0541353874522699
10.1842010591256997	2.0368402345401031	10.0541354017379483
8.1473608615608466	2.0368402260854372	12.1149730377933746
10.1842010448399609	0.0000000142857475	12.1149730605488291
8.1473608473005577	6.1105206354499702	7.9932977455807785
10.1842010733859887	4.0736804379105687	7.9932977598665387
8.1473608245855953	4.0736804463652430	10.0541354017379483
10.1842010591256997	6.1105206211896812	10.0541353874522397
8.1473608388458825	6.1105206212151302	12.1149730293236608
10.1842010448654108	4.0736804236248298	12.1149730293236626
8.1473608473005577	10.1842010591256997	7.9932977085396173
10.1842010591256997	8.1473608187545317	7.9932977312950699
8.1473608473005577	8.1473608245855971	10.0541353874522699
10.1842010591256997	10.1842010448654108	10.0541353874522095
8.1473608245855953	10.1842010591256997	12.1149730663648576
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8.1473608473005577	14.2578814827759786	7.9932976857841629
10.1842010591256997	12.2210412566905511	7.9932976857841629

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  8.1473608473005577 12.2210412482358777 10.0541353874522397
 10.1842010591256997 14.2578814827759786 10.0541353874522397
  8.1473608473005577 14.2578814828014284 12.1149730891203120
 10.1842010818406621 12.2210412852365788 12.1149730891203120

Interface: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Cu E_tot= -687.4905187 eV
 D3-zero damping= -43.5234953 eV, D3-BJ damping= -51.2996431 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Cu
 1.0000000000000000
    10.7074477457069577    0.0000000000000000    0.0000000000000000
     0.0000000000000000   14.2765969942759412    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.8911664483577368
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2  72
Selective dynamics
Cartesian
  3.5692834317119968  0.0044505757789790  8.0000000000000000   F   F   F
  1.7847079734028926  2.3838834131942810  8.0000055199296671   F   F   F
  3.5692833293502635  1.8086772360580852  8.0000008619369254   F   F   F
  1.7847086520056328  4.1881100762768710  8.0000049280612373   F   F   F
  0.8924163624334334  0.0044505931882727  9.6370125635575068   F   F   F
  4.4615647769778084  2.3838834306035745  9.6370180834871757   F   F   F
  0.8924162600716995  1.8086772534673790  9.6370134254944340   F   F   F
  4.4615654555805486  4.1881100936861637  9.6370174916187459   F   F   F
  3.6899966929225130 -0.1110412747020401 11.4676636045781386   T   T   T
  1.6982165537012806  2.2137707415756203 11.4438597580969574   T   T   T
  3.6546192338594743  1.8859417249996575 11.4336705600222253   T   T   T
  1.7020684791688743  4.2039524450167498 11.3931781159537557   T   T   T
  0.9523173165801024 -0.0840750285718176 13.2320822852259141   T   T   T
  4.3841914396872035  2.1722719343792756 13.2379305096854321   T   T   T
  0.8573712345886463  1.9436081064268111 13.2166515963084716   T   T   T
  4.3110599116089778  4.2369542525743871 13.3018666024386043   T   T   T
  3.5692835846082009  4.7633162405376233  8.0000000000000000   F   F   F
  1.7847081262990971  7.1427490779529252  8.0000055199296671   F   F   F
  3.5692834822464685  6.5675429008167301  8.0000008619369254   F   F   F
  1.7847088049018380  8.9469757410355157  8.0000049280612373   F   F   F
  0.8924165153296379  4.7633162579469177  9.6370125635575068   F   F   F
  4.4615649298740125  7.1427490953622197  9.6370180834871757   F   F   F
  0.8924164129679044  6.5675429182260245  9.6370134254944340   F   F   F
  4.4615656084767528  8.9469757584448075  9.6370174916187459   F   F   F
  3.6414957744034644  4.5868549642417564 11.4455409919725959   T   T   T
  1.7209733256747002  6.9917787089284085 11.3855241621996655   T   T   T
  3.6431088182587779  6.5700426090648794 11.3914288326785158   T   T   T
  1.7299362603050332  8.9783653901953926 11.3801016314057417   T   T   T
  0.9783897244932375  4.5126977854464423 13.1795899135317249   T   T   T
  4.1374828712153180  7.0471068896642715 13.2178389627412525   T   T   T
  0.9848006121010826  6.5540466792592298 13.1506814153245273   T   T   T
  4.3443095502024303  9.0574957720880871 13.1159884591204996   T   T   T
  3.5692837375044064  9.5221819052962697  8.0000000000000000   F   F   F
  1.7847082791953022 11.9016147427115708  8.0000055199296671   F   F   F
  3.5692836351426735 11.3264085655753757  8.0000008619369254   F   F   F
  1.7847089577980424 13.7058414057941604  8.0000049280612373   F   F   F
  0.8924166682258426  9.5221819227055633  9.6370125635575068   F   F   F
  4.4615650827702176 11.9016147601208626  9.6370180834871757   F   F   F
  0.8924165658641090 11.3264085829846710  9.6370134254944340   F   F   F
  4.4615657613729578 13.7058414232034522  9.6370174916187459   F   F   F
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  3.6487462918739095 11.4509090158957978 11.4212854127065775   T   T   T
  1.7237720913249535 13.8222085904466319 11.4464188654292958   T   T   T
  1.1531344936791568  9.3526435263751466 13.1978206555403492   T   T   T
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4.4318937293463092	11.8080597093181421	13.1774331295992457	T	T	T
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8.9230073045654770	0.0044505757789790	8.0000000000000000	F	F	F
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7.1384325248591107	4.1881100762768710	8.0000049280612373	F	F	F
6.2461402352869104	0.0044505931882727	9.6370125635575068	F	F	F
9.8152886498312881	2.3838834306035745	9.6370180834871757	F	F	F
6.2461401329251780	1.8086772534673790	9.6370134254944340	F	F	F
9.8152893284340266	4.1881100936861637	9.6370174916187459	F	F	F
8.9869901115299857	-0.1467820531812863	11.3857372759688946	T	T	T
7.0755571488872508	2.3297141362626328	11.3560457690399144	T	T	T
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7.0590114436898341	4.3122045002023075	11.4212592496914240	T	T	T
6.5699133092816728	-0.0913230830635902	13.2178935700702329	T	T	T
9.5547427476199083	2.2143793974872148	13.1977707792876853	T	T	T
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9.8152888027274923	7.1427490953622197	9.6370180834871757	F	F	F
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9.7229088071820460	13.6919293113816529	13.1509723439932191	T	T	T
0.1215625408511524	1.7313927842312526	15.2653349398787128	T	T	T
1.8716052068274867	-0.0168296047006152	15.4677782350580451	T	T	T
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-0.0612552801017133	1.7754729092515946	18.8329967512973866	T	T	T
1.7629078480691096	-0.0083076262662922	18.8965732239168176	T	T	T
-0.0573037621068896	5.4042956019114152	15.2966338861785829	T	T	T
1.7891840012100515	3.5537715728402803	15.3167191238814322	T	T	T
-0.0164127712514034	3.5618427298934234	17.0340001929162668	T	T	T
1.8058877635666180	5.3854533189888008	16.9469258268430742	T	T	T
0.0401666234403480	5.3580249113288145	18.8111568141085890	T	T	T
1.7743821576931933	3.5848041401389579	18.8557524223150885	T	T	T

-0.1216285152623950	8.8697399674088686	15.2651911572869601	T	T	T
1.8159921821070657	7.1677786116584787	14.9369052760465824	T	T	T
0.0291692183589994	7.1473233023343532	17.0523157698000603	T	T	T
1.7959817339795796	8.9083599324351734	16.8640921900020295	T	T	T
0.0611699378462618	8.9136973571881946	18.8329946093578577	T	T	T
1.8290868604493813	7.1449030204464794	18.7280129537341686	T	T	T
0.0571662002817135	12.5425570793137116	15.2966230069202034	T	T	T
1.7965620617366425	10.7741264027908397	15.1343798633642077	T	T	T
0.0163263199858133	10.7001031124622141	17.0340431745345597	T	T	T
1.7783137997640615	12.4637023765260739	17.1253436957550491	T	T	T
-0.0403005996337801	12.4963029236052829	18.8112246761449775	T	T	T
1.7912293198735867	10.6791856395574225	18.8016005152360535	T	T	T
3.4772848380707657	1.7867460363980241	15.4517190305034919	T	T	T
5.1841096165284961	0.0365592623206774	15.2337737358069916	T	T	T
3.5956172644661395	-0.0127281948779994	17.1918311365405394	T	T	T
5.3776809134521493	1.7653577116325514	17.0335373884188606	T	T	T
3.5943918504668533	1.7927775446226932	18.8870927503979047	T	T	T
5.4199850237737222	-0.0013633790209347	18.8240417564708977	T	T	T
3.5556668162330749	5.3138293261403327	15.0271062179528574	T	T	T
5.3338505698564811	3.5456824688798081	15.2976226710229000	T	T	T
3.5643553647628110	3.5967292889570976	17.0826017545671327	T	T	T
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5.3670750687702151	3.5624041866086245	18.7969993355609368	T	T	T
3.5452405031742003	8.9732532779913878	15.0071526794614929	T	T	T
5.5233502841303830	7.1749122520397632	15.2337903090869649	T	T	T
3.5643529658977466	7.1348539169653122	16.8271616206746089	T	T	T
5.3296949273266820	8.9036420820725137	17.0335165528843930	T	T	T
3.5408919372185097	8.9042576488320790	18.7328028868882654	T	T	T
5.2874162303942951	7.1368770060702342	18.8239234334105632	T	T	T
3.5286344999845416	12.4936335215796959	15.3529323575318752	T	T	T
5.3734907892326671	10.6840560704713390	15.2977427930007970	T	T	T
3.5551325898888986	10.6774177546950408	16.9890679164028668	T	T	T
5.3814880427604761	12.5051419222179359	17.0200840152876900	T	T	T
3.5922824703240321	12.4641232722420572	18.8603366677699320	T	T	T
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7.1621518833597415	1.8348879513103793	15.0072978581032253	T	T	T
8.8914473233577596	0.0294529063569064	14.9369134318909182	T	T	T
7.1430461766455799	-0.0034417870113762	16.8272591304409538	T	T	T
8.9114074863028421	1.7700856329083956	16.8641245913791487	T	T	T
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7.1787515900094006	5.3552766401218790	15.3525280241458510	T	T	T
8.9108717711614087	3.6357556162499409	15.1343097208789743	T	T	T
7.1522211007288403	3.5391669218143558	16.9889562425313017	T	T	T
8.9289586024758520	5.3254250014387257	17.1251975648636652	T	T	T
7.1150600510251270	5.3258355519940226	18.8602366776653767	T	T	T
8.9161234085496837	3.5409434391606447	18.8015130442450591	T	T	T
7.2300691440019724	8.9251284298284208	15.4516295505386356	T	T	T
8.8357401644814093	7.1215126420641663	15.4675436049208415	T	T	T
7.1117918176485349	7.1255282488754510	17.1916462652227366	T	T	T
8.9507348879614970	8.9328130593982760	17.1847032040215808	T	T	T
7.1129740616343087	8.9309832256441553	18.8870444898911352	T	T	T
8.9444168667866055	7.1299507652815874	18.8965154913120017	T	T	T
7.1516540007691178	12.4521508229947138	15.0271389605902890	T	T	T
8.9181123447487618	10.6920721921660551	15.3168605271980507	T	T	T
7.1430026189525666	10.7350171101977914	17.0826747367536775	T	T	T
8.9014574366944856	12.5237487402622385	16.9469680115797878	T	T	T
7.1511664614908304	12.5103055267046486	18.7798699830148905	T	T	T
8.9329875666354432	10.7230368532585292	18.8557850602047594	T	T	T

Oxide reference: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Cu E_tot= -409.66812412 eV

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 D3-zero damping= -13.9563553 eV, D3-BJ damping= -16.2462405 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
    10.7074477457069577    0.0000000000000000    0.0000000000000000
     0.0000000000000000   14.2765969942759412    0.0000000000000000
     0.0000000000000000    0.0000000000000000   21.2660162450947823
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.5692834317119968  0.0044505757789790  8.0000000000000000   F   F   F
  1.7847079734028926  2.3838834131942810  8.0000055199296671   F   F   F
  3.5692833293502635  1.8086772360580852  8.0000008619369254   F   F   F
  1.7847086520056328  4.1881100762768710  8.0000049280612373   F   F   F
  0.8924163624334334  0.0044505931882727  9.6370125635575068   F   F   F
  4.4615647769778084  2.3838834306035745  9.6370180834871757   F   F   F
  0.8924162600716995  1.8086772534673790  9.6370134254944340   F   F   F
  4.4615654555805486  4.1881100936861637  9.6370174916187459   F   F   F
  3.6306714177347064 -0.1268378558454527 11.4480748271284973   T   T   T
  1.7203518510385998  2.2487609820676777 11.4474174543901785   T   T   T
  3.6570378436685691  1.8543166161755786 11.4065634107563358   T   T   T
  1.6988870214393157  4.2299464120842538 11.4045108176933674   T   T   T
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  3.5692835846082009  4.7633162405376233  8.0000000000000000   F   F   F
  1.7847081262990971  7.1427490779529252  8.0000055199296671   F   F   F
  3.5692834822464685  6.5675429008167301  8.0000008619369254   F   F   F
  1.7847088049018380  8.9469757410355157  8.0000049280612373   F   F   F
  0.8924165153296379  4.7633162579469177  9.6370125635575068   F   F   F
  4.4615649298740125  7.1427490953622197  9.6370180834871757   F   F   F
  0.8924164129679044  6.5675429182260245  9.6370134254944340   F   F   F
  4.4615656084767528  8.9469757584448075  9.6370174916187459   F   F   F
  3.6329932044227404  4.6314840741943826 11.4487842874570696   T   T   T
  1.7234342531177245  7.0115690133552784 11.4479716166988617   T   T   T
  3.6594017662207352  6.6146178338638180 11.4088164269505210   T   T   T
  1.6973209922023977  8.9926907828879159 11.4065102362853938   T   T   T
  0.8169273016987049  4.7501077004266676 13.0748201135820885   T   T   T
  4.5462414197217047  7.1338007238296548 13.0796643511612682   T   T   T
  1.0486908513250546  6.6453288022257846 13.2717839794969965   T   T   T
  4.3110989890950284  9.0294284435165384 13.2722906669924363   T   T   T
  3.5692837375044064  9.5221819052962697  8.0000000000000000   F   F   F
  1.7847082791953022 11.9016147427115708  8.0000055199296671   F   F   F
  3.5692836351426735 11.3264085655753757  8.0000008619369254   F   F   F
  1.7847089577980424 13.7058414057941604  8.0000049280612373   F   F   F
  0.8924166682258426  9.5221819227055633  9.6370125635575068   F   F   F
  4.4615650827702176 11.9016147601208626  9.6370180834871757   F   F   F
  0.8924165658641090 11.3264085829846710  9.6370134254944340   F   F   F
  4.4615657613729578 13.7058414232034522  9.6370174916187459   F   F   F
  3.6341649489404735  9.3870075906220602 11.4476334695515956   T   T   T
  1.7212815535497443 11.7696581664800792 11.4486625559812989   T   T   T
  3.6555276250234376 11.3681491773637209 11.4046261229503845   T   T   T
  1.6948295904015946 13.7528227703634602 11.4086833677037784   T   T   T
  0.8156569941204895  9.5126021976862596 13.0767252057436600   T   T   T
  4.5377323626245838 11.8883485983339394 13.0748087951795853   T   T   T
  1.0430855747817223 11.4081941213313804 13.2718639722777088   T   T   T
  4.3057767480455205 13.7835579294256227 13.2717924440062465   T   T   T
  8.9230073045654770  0.0044505757789790  8.0000000000000000   F   F   F
  7.1384318462563723  2.3838834131942810  8.0000055199296671   F   F   F
  8.9230072022037437  1.8086772360580852  8.0000008619369254   F   F   F
```

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  7.1384325248591107  4.1881100762768710  8.0000049280612373   F   F   F
  6.2461402352869104  0.0044505931882727  9.6370125635575068   F   F   F
  9.8152886498312881  2.3838834306035745  9.6370180834871757   F   F   F
  6.2461401329251780  1.8086772534673790  9.6370134254944340   F   F   F
  9.8152893284340266  4.1881100936861637  9.6370174916187459   F   F   F
  8.9843951405632119 -0.1268380735160898 11.4480748108709811   T   T   T
  7.0740756182551472  2.2487620885538218 11.4474182957198867   T   T   T
  9.0107617523803629  1.8543163324442797 11.4065631662918072   T   T   T
  7.0526103421497650  4.2299476409671311 11.4045121979421502   T   T   T
  6.1620528468031610 -0.0045866537564078 13.0797082465966898   T   T   T
  9.8928379649653202  2.3742978031643038 13.0765925948058026   T   T   T
  6.3972992668203261  1.8909860349390661 13.2721430291160303   T   T   T
  9.6653774045471614  4.2698607074741295 13.2718527407865814   T   T   T
  8.9230074574616793  4.7633162405376233  8.0000000000000000   F   F   F
  7.1384319991525773  7.1427490779529252  8.0000055199296671   F   F   F
  8.9230073550999460  6.5675429008167301  8.0000008619369254   F   F   F
  7.1384326777553158  8.9469757410355157  8.0000049280612373   F   F   F
  6.2461403881831163  4.7633162579469177  9.6370125635575068   F   F   F
  9.8152888027274923  7.1427490953622197  9.6370180834871757   F   F   F
  6.2461402858213839  6.5675429182260245  9.6370134254944340   F   F   F
  9.8152894813302325  8.9469757584448075  9.6370174916187459   F   F   F
  8.9867167458268256  4.6314845718522797 11.4487838578858483   T   T   T
  7.0771613594326874  7.0115726348059697 11.4479650317395336   T   T   T
  9.0131287010775285  6.6146186274590999 11.4088187340488929   T   T   T
  7.0510454912670388  8.9926939048865950 11.4065089607197319   T   T   T
  6.1706501883996889  4.7501207770221914 13.0748182359437699   T   T   T
  9.8999765790989809  7.1337973569682740 13.0796652186824094   T   T   T
  6.4024094076844351  6.6453379000614961 13.2717774669279720   T   T   T
  9.6648253075777308  9.0294242581556912 13.2722900088104865   T   T   T
  8.9230076103578835  9.5221819052962697  8.0000000000000000   F   F   F
  7.1384321520487823 11.9016147427115708  8.0000055199296671   F   F   F
  8.9230075079961519 11.3264085655753757  8.0000008619369254   F   F   F
  7.1384328306515208 13.7058414057941604  8.0000049280612373   F   F   F
  6.2461405410793214  9.5221819227055633  9.6370125635575068   F   F   F
  9.8152889556236946 11.9016147601208626  9.6370180834871757   F   F   F
  6.2461404387175881 11.3264085829846710  9.6370134254944340   F   F   F
  9.8152896342264366 13.7058414232034522  9.6370174916187459   F   F   F
  8.9878895751081043  9.3870069998607395 11.4476343009977963   T   T   T
  7.0750054989461431 11.7696578289610354 11.4486626026582865   T   T   T
  9.0092519609606629 11.3681489885203106 11.4046264806263089   T   T   T
  7.0485536231316610 13.7528224577786027 11.4086831335119143   T   T   T
  6.1693805958803418  9.5126002106599170 13.0767250369526202   T   T   T
  9.8914557940946040 11.8883485351407145 13.0748089274489470   T   T   T
  6.3968094928360486 11.4081931593383334 13.2718637940377562   T   T   T
  9.6595005838789945 13.7835579139747999 13.2717927462742189   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Cu E_tot= -260.96626049
eV
 D3-zero damping= -20.574761 eV, D3-BJ damping= -26.0467087 eV
Cu
 1.0000000000000000
    10.7074477457069577    0.0000000000000000    0.0000000000000000
     0.0000000000000000   14.2765969942759412    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.5821021653327065
  72
Cartesian
  0.0000000000000000  1.7844946726630631  7.9958921784754029
  1.7845746242844938  0.0000000000000000  7.9947881939809271
 -0.0000000000000000  0.0000002998245459  9.7910510771445889
  1.7845746242844938  1.7844920449420025  9.7910514170520457
 -0.0000000000000000  1.7844948316887328 11.5862102994579228
  1.7845746242844938 -0.0000000000000000 11.5873139844238917
 -0.0000000000000000  5.3538038244749240  7.9958921546558201
```

1.7845746242844938	3.5691492485689853	7.9949254447574916
-0.0000000000000000	3.5691492629225419	9.7910510627910412
1.7845746242844938	5.3538064503007128	9.7910510386642589
0.0000000000000000	5.3538035487342306	11.5862099614490930
1.7845746242844938	3.5691492485689853	11.5871767336584668
0.0000000000000000	8.9227931457171685	7.9958918835495263
1.7845746242844938	7.1382984971379706	7.9947885081701617
0.0000000000000000	7.1382982116525691	9.7910510771445889
1.7845746242844938	8.9227899586652946	9.7910511172275001
0.0000000000000000	8.9227931457171685	11.5862102850932178
1.7845746242844938	7.1382984971379706	11.5873136604725637
0.0000000000000000	12.4921023456967433	7.9958915550067280
1.7845746242844938	10.7074477457069559	7.9949251208061645
-0.0000000000000000	10.7074477313534082	9.7910510771445889
1.7845746242844938	12.4921052491584650	9.7910510386642589
-0.0000000000000000	12.4921021863644057	11.5862102994579228
1.7845746242844938	10.7074477457069559	11.5871770191183074
3.5691492485689875	1.7844949724876089	7.9958922026021817
5.3537238728534788	0.0000000000000000	7.9947881796273794
3.5691492485689875	0.0000002998245459	9.7910510627910412
5.3537238728534788	1.7844921090374437	9.7910511077726188
3.5691492485689875	1.7844946726630631	11.5862102899918895
5.3537238728534788	-0.0000000000000000	11.5873139602971094
3.5691492485689875	5.3538035246503783	7.9958921784753993
5.3537238728534788	3.5691492485689853	7.9949255339076410
3.5691492485689875	3.5691492485689853	9.7910510771445889
5.3537238728534788	5.3538064024396652	9.7910510386642589
3.5691492485689875	5.3538038244749240	11.5862099758137980
5.3537238728534788	3.5691492485689853	11.5871766347350835
3.5691492485689875	8.9227931457171685	7.9958918933116037
5.3537238728534788	7.1382984971379706	7.9947885081701617
3.5691492485689875	7.1382981973134250	9.7910510771445889
5.3537238728534788	8.9227902279162681	9.7910511077726188
3.5691492485689875	8.9227931457171685	11.5862102961478666
5.3537238728534788	7.1382984971379706	11.5873136604725637
3.5691492485689875	12.4921023456967433	7.9958915550067280
5.3537238728534788	10.7074477457069559	7.9949251208061645
3.5691492342298368	10.7074477313534082	9.7910510771445889
5.3537238728534788	12.4921052329240698	9.7910510386642589
3.5691492485689875	12.4921023456967433	11.5862102753311405
5.3537238728534788	10.7074477457069559	11.5871770334830124
7.1382984971379706	1.7844948316887328	7.9958921784753993
8.9228731214224677	-0.0000000000000000	7.9947881939809271
7.1382984971379706	0.0000002998245458	9.7910510530289585
8.9228731214224677	1.7844919169684335	9.7910510934079209
7.1382984971379706	1.7844946726630631	11.5862102994579228
8.9228731214224677	-0.0000000000000000	11.5873139602971094
7.1382984971379706	5.3538038244749240	7.9958918548312745
8.9228731214224677	3.5691492485689853	7.9949252178197634
7.1382984971379706	3.5691492629225419	9.7910510771445889
8.9228731214224677	5.3538064262168623	9.7910509985813476
7.1382984971379706	5.3538036654492425	11.5862099470955080
8.9228731214224677	3.5691492485689853	11.5871767480120145
7.1382984971379706	8.9227931457171685	7.9958918930044005
8.9228731214224677	7.1382984971379706	7.9947882083456161
7.1382984971379706	7.1382981973134250	9.7910510771445889
8.9228731357616073	8.9227902422554468	9.7910513932324665
7.1382984971379706	8.9227934455417142	11.5862102994579228
8.9228731214224677	7.1382984971379706	11.5873136604725637
7.1382984971379706	12.4921021625872104	7.9958915550067280
8.9228731357616073	10.7074477457069559	7.9949251351597121
7.1382984971379706	10.7074477313534082	9.7910510915092885
8.9228731214224677	12.4921052491584650	9.7910510386642589

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  7.1382984971379706 12.4921023456967433 11.5862102994579228
  8.9228731214224677 10.7074477457069559 11.5871770334830124

Interface: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Pt E_tot= -871.4517937 eV
 D3-zero damping= -59.3020703 eV, D3-BJ damping= -58.1520187 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Pt
 1.0000000000000000
    11.7540381698974450    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.6720508931965945    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.8077535370500541
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2  72
Selective dynamics
Cartesian
  3.9181600220599888  0.0048855935444667  8.0000000000000000   F   F   F
  1.9591527448647730  2.6168940812721155  8.0000055199296671   F   F   F
  3.9181599096929944  1.9854648628264409  8.0000008619369254   F   F   F
  1.9591534897969642  4.5974733536315968  8.0000049280612373   F   F   F
  0.9796448450275431  0.0048856126554171  9.6370125635575068   F   F   F
  4.8976566527810492  2.6168941003830652  9.6370180834871757   F   F   F
  0.9796447326605481  1.9854648819373915  9.6370134254944340   F   F   F
  4.8976573977132407  4.5974733727425470  9.6370174916187459   F   F   F
  3.9125136440446417  0.0444738913711168 11.3367050030560961   T   T   T
  1.9620202174192316  2.5513821398970720 11.3295725209814311   T   T   T
  3.8934315943923514  2.0440365471247346 11.3339789405738198   T   T   T
  1.9166058962332817  4.5465979100109273 11.2906488018138731   T   T   T
  0.9916227894359798 -0.2126496707837429 12.9720720071126383   T   T   T
  4.8476973473774292  2.6855619206105485 12.9861253510407177   T   T   T
  0.7388652044960011  1.8165274242757776 12.7149591841511960   T   T   T
  4.8919318298488923  4.7030662599529789 12.7745471446550898   T   T   T
  3.9181601899009033  5.2289025579433286  8.0000000000000000   F   F   F
  1.9591529127056879  7.8409110456709765  8.0000055199296671   F   F   F
  3.9181600775339094  7.2094818272253027  8.0000008619369254   F   F   F
  1.9591536576378796  9.8214903180304614  8.0000049280612373   F   F   F
  0.9796450128684578  5.2289025770542787  9.6370125635575068   F   F   F
  4.8976568206219655  7.8409110647819285  9.6370180834871757   F   F   F
  0.9796449005014631  7.2094818463362547  9.6370134254944340   F   F   F
  4.8976575655541561  9.8214903371414071  9.6370174916187459   F   F   F
  3.7971466565077598  5.1886664939378786 11.2213471604787927   T   T   T
  1.9965799300182503  7.8469415058380259 11.1820000045142329   T   T   T
  3.8366775367545509  7.1751263546603159 11.1606138220699211   T   T   T
  2.0348310167600361  9.8193865385118180 11.2255540318832985   T   T   T
  0.9207772628170355  5.0401419799010032 12.9227626686869321   T   T   T
  4.6370661830318429  7.8341183837523580 12.7965525460490728   T   T   T
  0.9268331475950905  7.0978025740867512 12.6537405821476483   T   T   T
  4.9937575452234269  9.8198873324428568 12.6483620408684168   T   T   T
  3.9181603577418187 10.4529195223421922  8.0000000000000000   F   F   F
  1.9591530805466031 13.0649280100698402  8.0000055199296671   F   F   F
  3.9181602453748248 12.4334987916241673  8.0000008619369254   F   F   F
  1.9591538254787946 15.0455072824293214  8.0000049280612373   F   F   F
  0.9796451807093728 10.4529195414531415  9.6370125635575068   F   F   F
  4.8976569884628791 13.0649280291807894  9.6370180834871757   F   F   F
  0.9796450683423780 12.4334988107351183  9.6370134254944340   F   F   F
  4.8976577333950706 15.0455073015402707  9.6370174916187459   F   F   F
  3.8809055684616256 10.5251229259059400 11.1948310176021408   T   T   T
  2.0193144732949273 13.0568482821071381 11.2550192628952139   T   T   T
  3.9313141284385700 12.4972912248067107 11.3179587553620244   T   T   T
  2.0063423072744095 15.0473338287587133 11.3094092149227752   T   T   T
  1.2038651909118749 10.1703491472499579 12.9647894708667959   T   T   T
  4.8808708868057025 13.0590075595859965 12.9566528016887119   T   T   T
  0.9943217579424541 12.2107151032684982 12.7273117583148370   T   T   T
```

5.1298991490137764	15.0688300625218492	12.7368277766720173	T	T	T
9.7951791070087104	0.0048855935444667	8.0000000000000000	F	F	F
7.8361718298134955	2.6168940812721155	8.0000055199296671	F	F	F
9.7951789946417183	1.9854648628264409	8.0000008619369254	F	F	F
7.8361725747456852	4.5974733536315968	8.0000049280612373	F	F	F
6.8566639299762642	0.0048856126554171	9.6370125635575068	F	F	F
10.7746757377297744	2.6168941003830652	9.6370180834871757	F	F	F
6.8566638176092702	1.9854648819373915	9.6370134254944340	F	F	F
10.7746764826619632	4.5974733727425470	9.6370174916187459	F	F	F
9.7577233843820554	0.0109016303256223	11.1819063585084457	T	T	T
7.8734029899956566	2.6890457695647352	11.1948626304911194	T	T	T
9.7194475274157135	1.9833354014633708	11.2255045711013928	T	T	T
7.8231044177221190	4.6612613597760468	11.3177815333526208	T	T	T
7.1170927859155571	-0.0022210989559662	12.7963324840744974	T	T	T
10.5505868311684736	2.3339424841203984	12.9647190535078174	T	T	T
6.7606616555979810	1.9838048841752434	12.6484624093270561	T	T	T
10.7597963772877261	4.3743903948596135	12.7271743863889419	T	T	T
9.7951792748496267	5.2289025579433286	8.0000000000000000	F	F	F
7.8361719976544117	7.8409110456709765	8.0000055199296671	F	F	F
9.7951791624826292	7.2094818272253027	8.0000008619369254	F	F	F
7.8361727425866006	9.8214903180304614	8.0000049280612373	F	F	F
6.8566640978171787	5.2289025770542787	9.6370125635575068	F	F	F
10.7746759055706871	7.8409110647819285	9.6370180834871757	F	F	F
6.8566639854501865	7.2094818463362547	9.6370134254944340	F	F	F
10.7746766505028777	9.8214903371414071	9.6370174916187459	F	F	F
9.7350789089470435	5.2207354566473088	11.2548992203713638	T	T	T
7.8417984884690348	7.8805890847122706	11.3367000417350088	T	T	T
9.7478890454826193	7.2112509805187441	11.3092527138314729	T	T	T
7.8611591765280009	9.8801473658504584	11.3338883294785528	T	T	T
6.8735182939235653	5.2232882839652168	12.9563290447296637	T	T	T
10.7625128820349953	7.6232566463542106	12.9719237969634946	T	T	T
6.6244873286349435	7.2331410805714649	12.7365844881628263	T	T	T
11.0157288820162336	9.6523319613060323	12.7148356841135968	T	T	T
9.7951794426905394	10.4529195223421922	8.0000000000000000	F	F	F
7.8361721654953271	13.0649280100698402	8.0000055199296671	F	F	F
9.7951793303235473	12.4334987916241673	8.0000008619369254	F	F	F
7.8361729104275160	15.0455072824293214	8.0000049280612373	F	F	F
6.8566642656580949	10.4529195414531415	9.6370125635575068	F	F	F
10.7746760734116016	13.0649280291807894	9.6370180834871757	F	F	F
6.8566641532911001	12.4334988107351183	9.6370134254944340	F	F	F
10.7746768183437940	15.0455073015402707	9.6370174916187459	F	F	F
9.7926454677170334	10.3874698632445170	11.3295606221989882	T	T	T
7.9573368909953066	13.0244748924532292	11.2211705900058174	T	T	T
9.8379233979603349	12.3826972758962892	11.2907866575767031	T	T	T
7.9177100711386972	15.0109259599952996	11.1604524089152370	T	T	T
6.9068782884730533	10.5215809031243470	12.9859452074581867	T	T	T
10.8332926371053588	12.8765653820769863	12.9231901855195090	T	T	T
6.8627584525284577	12.5390046730847917	12.7744205058098750	T	T	T
10.8272322792664646	14.9342741452562144	12.6540620373585835	T	T	T
1.0544036515387911	2.1111459993670922	14.7479598360098709	T	T	T
2.0762143710017642	-0.2240757231748548	15.2665430740678385	T	T	T
-0.0976396898250479	0.1357196201649286	17.0488151901201057	T	T	T
2.0162442185544114	1.8075211106711151	17.2313583794174150	T	T	T
0.0162747311003549	1.8363994913844581	19.0412908343514786	T	T	T
1.9208683330997947	-0.3099932809939098	18.9927990552204200	T	T	T
0.0882441244367730	5.9902436950186830	15.3031469272263578	T	T	T
2.2242663415756092	4.3935697525154245	15.0499283902333012	T	T	T
0.0619701165901628	3.6326713979346614	16.8593796423861058	T	T	T
2.0445794966676005	6.0486948372670133	17.0967165615481846	T	T	T
0.0347895116505111	5.6509602838413882	18.9024535233982363	T	T	T
1.9434656471394882	3.8268880346584249	18.9968560288323829	T	T	T
-1.0536093109736864	9.9465628037787717	14.7480263271711323	T	T	T
2.1884796040241525	7.4576434924262465	14.2991448292834757	T	T	T

0.0976638076264806	7.9717944868057815	17.0488365050484667	T	T	T
1.4847381742964261	9.6814727937661971	15.5628724597670338	T	T	T
-0.0162650755819383	9.6723193585701512	19.0416579842430025	T	T	T
1.8382364560467934	7.7381867802132343	19.0913307998735817	T	T	T
-0.0883551206854985	13.8259351448609227	15.3033353841367727	T	T	T
1.9209027231953162	12.2190958799437261	14.6024838828891905	T	T	T
-0.0607809500966871	11.4675676528105530	16.8595689724030215	T	T	T
1.8805208166185496	13.4567319757820130	17.0437729562827549	T	T	T
-0.0346715683538723	13.4869830988548323	18.9024303273141321	T	T	T
1.8800451524602240	11.4280712446710240	18.8231804767213902	T	T	T
3.7589943149355465	2.0305410542610005	15.1754306283657083	T	T	T
5.4261465058944456	0.0267163671037498	14.7490745310358413	T	T	T
3.9824477191884431	-0.1248617928617726	17.2358414913707385	T	T	T
5.9633316611815275	1.6557953836332764	16.8374622184394660	T	T	T
4.0906914280048419	1.8463017758032745	19.0431394035669186	T	T	T
6.0598104858855493	-0.0735984561464017	18.9785006021114810	T	T	T
4.3606131788975322	5.8484376840739269	14.5153916410848627	T	T	T
5.8993665295212798	3.8386585587578579	15.3626140987816910	T	T	T
3.8815756783049129	3.8797537210987745	17.1625516954490820	T	T	T
5.7039731868613819	5.8729901445621984	17.1414113144278915	T	T	T
3.8155676735092290	5.8500607595447800	19.0381202732671255	T	T	T
6.1102715719807659	3.5984967192791917	18.7172232559268714	T	T	T
3.9373429896292751	10.0384535168505771	14.4481320942786660	T	T	T
6.3291726326058289	7.8630688778529985	14.7487949317683924	T	T	T
3.8314649365716025	7.7587440799880900	16.2631088414450602	T	T	T
5.7910544867718308	9.4920004753966793	16.8369349944746922	T	T	T
3.6966065475226393	9.4326970785360142	18.6235561576879007	T	T	T
5.6942623572567381	7.7626028859420764	18.9784207669004559	T	T	T
4.0242013847580713	13.5935879854460744	15.3332816584162490	T	T	T
5.8552714183421850	11.6752197664200779	15.3626185837888638	T	T	T
3.5556370075195778	11.2882952386764579	16.7518008125847260	T	T	T
6.0501085275562581	13.7089371921115433	17.1413752307907714	T	T	T
3.8488478496283993	13.3233926737091029	18.8307866703094255	T	T	T
5.6437276007908688	11.4343355514387355	18.7174026087053775	T	T	T
7.8168195508087965	2.2006298286829313	14.4485385694011654	T	T	T
9.5657909159833725	-0.3773944802761568	14.2993655382348805	T	T	T
7.9227635502087557	-0.0776570024833260	16.2632978180078354	T	T	T
10.2704699782977116	1.8465924540116436	15.5625892236000709	T	T	T
8.0575688593234620	1.5968036817635292	18.6235802438903448	T	T	T
9.9159734326610831	-0.0977305037775513	19.0910757014955728	T	T	T
7.7297608282316910	5.7572266521734932	15.3332657054825567	T	T	T
9.8333866712429714	4.3832590500806452	14.6022069713009106	T	T	T
8.1990039845287424	3.4519914275645953	16.7516244475868206	T	T	T
9.8737942608964477	5.6206672833486264	17.0433030750389491	T	T	T
7.9054858034612669	5.4872874508936711	18.8305775594493241	T	T	T
9.8744040430721682	3.5920303104548754	18.8226646831325048	T	T	T
7.9961066446629010	9.8671017075151042	15.1751805667312798	T	T	T
9.6775810092868841	7.6116625991980014	15.2661114259907738	T	T	T
7.7718082166519835	7.7111654075913654	17.2359244254328701	T	T	T
9.7381711441531351	9.6435138353054306	17.2315303360759842	T	T	T
7.6632307756233304	9.6821949069624722	19.0431790865643578	T	T	T
9.8336300105736942	7.5257627761361068	18.9925840671112134	T	T	T
7.3947714633384152	13.6840006530180123	14.5151577296202987	T	T	T
9.5305207856181120	12.2286572417624217	15.0502919217189479	T	T	T
7.8724882675753429	11.7154982270656358	17.1626709832706794	T	T	T
9.7095146143444993	13.8844465919085760	17.0966157051801559	T	T	T
7.9386498117833826	13.6860126748927762	19.0382173347864949	T	T	T
9.8108226447190212	11.6629995745764443	18.9968320923933938	T	T	T

Oxide reference: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Pt E_tot= -417.57431452 eV
D3-zero damping= -12.5570352 eV, D3-BJ damping= -14.0725918 eV

```
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
    11.7540381698974450    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.6720508931965945    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.8659227569539993
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.9181600220599888  0.0048855935444667  7.9999999999999991   F   F   F
  1.9591527448647730  2.6168940812721155  8.0000055199296654   F   F   F
  3.9181599096929944  1.9854648628264409  8.0000008619369254   F   F   F
  1.9591534897969642  4.5974733536315968  8.0000049280612373   F   F   F
  0.9796448450275431  0.0048856126554171  9.6370125635575050   F   F   F
  4.8976566527810492  2.6168941003830652  9.6370180834871739   F   F   F
  0.9796447326605481  1.9854648819373915  9.6370134254944340   F   F   F
  4.8976573977132407  4.5974733727425470  9.6370174916187459   F   F   F
  3.8662918419904111 -0.0084221256031543 11.3121079664084068   T   T   T
  2.0115414247347507  2.6037606546030356 11.3118946234705255   T   T   T
  3.9098277953237188  1.9944407690818495 11.2949689258761730   T   T   T
  1.9688960429330249  4.6063371584378823 11.2952159166428761   T   T   T
  0.7400066752993392  0.1325545138182853 12.6398857395428195   T   T   T
  5.1387166284053984  2.7456296552234192 12.6359765119947784   T   T   T
  0.9895894097353028  1.9921660749364143 12.8774770512448544   T   T   T
  4.8899614956590787  4.6050089738780837 12.8768686917115769   T   T   T
  3.9181601899009033  5.2289025579433286  7.9999999999999991   F   F   F
  1.9591529127056879  7.8409110456709765  8.0000055199296654   F   F   F
  3.9181600775339094  7.2094818272253027  8.0000008619369254   F   F   F
  1.9591536576378796  9.8214903180304614  8.0000049280612373   F   F   F
  0.9796450128684578  5.2289025770542787  9.6370125635575050   F   F   F
  4.8976568206219655  7.8409110647819285  9.6370180834871739   F   F   F
  0.9796449005014631  7.2094818463362547  9.6370134254944340   F   F   F
  4.8976575655541561  9.8214903371414071  9.6370174916187459   F   F   F
  3.8677323983705607  5.2172414841354655 11.3118652810427278   T   T   T
  2.0108007996592367  7.8276317482387583 11.3121379857275244   T   T   T
  3.9095178480473884  7.2185841252693468 11.2954730467848758   T   T   T
  1.9672966660998077  9.8304551041177302 11.2950138685788684   T   T   T
  0.7426680486055955  5.3559550662980069 12.6396080572623859   T   T   T
  5.1370586545370323  7.9684794861754300 12.6399059354945180   T   T   T
  0.9888072542103884  7.2159508025011432 12.8778233250586300   T   T   T
  4.8874687068438973  9.8280824049684163 12.8775156811555558   T   T   T
  3.9181603577418187 10.4529195223421922  7.9999999999999991   F   F   F
  1.9591530805466031 13.0649280100698402  8.0000055199296654   F   F   F
  3.9181602453748248 12.4334987916241673  8.0000008619369254   F   F   F
  1.9591538254787946 15.0455072824293214  8.0000049280612373   F   F   F
  0.9796451807093728 10.4529195414531415  9.6370125635575050   F   F   F
  4.8976569884628791 13.0649280291807894  9.6370180834871739   F   F   F
  0.9796450683423780 12.4334988107351183  9.6370134254944340   F   F   F
  4.8976577333950706 15.0455073015402707  9.6370174916187459   F   F   F
  3.8655780658493057 10.4397096676214680 11.3118369356666211   T   T   T
  2.0094537258716980 13.0531837345079751 11.3119696167948280   T   T   T
  3.9083058061389191 12.4422516274137855 11.2951896882294509   T   T   T
  1.9675414425565854 15.0545738017792310 11.2956027276685109   T   T   T
  0.7384076638015425 10.5814613969939586 12.6360665969946577   T   T   T
  5.1346276079960163 13.1918675922013993 12.6396008594660643   T   T   T
  0.9872279791687349 12.4408252921563367 12.8770213209463211   T   T   T
  4.8882840227308471 15.0518783076778995 12.8777397059852099   T   T   T
  9.7951791070087104  0.0048855935444667  7.9999999999999991   F   F   F
  7.8361718298134955  2.6168940812721155  8.0000055199296654   F   F   F
  9.7951789946417183  1.9854648628264409  8.0000008619369254   F   F   F
  7.8361725747456852  4.5974733536315968  8.0000049280612373   F   F   F
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  6.8566639299762642  0.0048856126554171  9.6370125635575050   F   F   F
 10.7746757377297744  2.6168941003830652  9.6370180834871739   F   F   F
  6.8566638176092702  1.9854648819373915  9.6370134254944340   F   F   F
 10.7746764826619632  4.5974733727425470  9.6370174916187459   F   F   F
  9.7433106590366627 -0.0084225167139579 11.3121087555191462   T   T   T
  7.8885603353531417  2.6037597609930043 11.3118948515157385   T   T   T
  9.7868468339482071  1.9944400329259624 11.2949687528521832   T   T   T
  7.8459149936368231  4.6063374382899180 11.2952154026494682   T   T   T
  6.6170252597177717  0.1325536588145555 12.6398854732891621   T   T   T
 11.0157353808188159  2.7456290645622103 12.6359760706889883   T   T   T
  6.8666085260462202  1.9921650465660485 12.8774767372460843   T   T   T
 10.7669793350750922  4.6050093368515306 12.8768687007075489   T   T   T
  9.7951792748496267  5.2289025579433286  7.9999999999999991   F   F   F
  7.8361719976544117  7.8409110456709765  8.0000055199296654   F   F   F
  9.7951791624826292  7.2094818272253027  8.0000008619369254   F   F   F
  7.8361727425866006  9.8214903180304614  8.0000049280612373   F   F   F
  6.8566640978171787  5.2289025770542787  9.6370125635575050   F   F   F
 10.7746759055706871  7.8409110647819285  9.6370180834871739   F   F   F
  6.8566639854501865  7.2094818463362547  9.6370134254944340   F   F   F
 10.7746766505028777  9.8214903371414071  9.6370174916187459   F   F   F
  9.7447506365236212  5.2172396605376692 11.3118643006875299   T   T   T
  7.8878129174885263  7.8276330647082757 11.3121360409929093   T   T   T
  9.7865327355149248  7.2185854737263160 11.2954763775036273   T   T   T
  7.8442824791147707  9.8304598681867166 11.2950413430019552   T   T   T
  6.6196859085860158  5.3559575293621933 12.6396071176039673   T   T   T
 11.0140760728274305  7.9684573259995650 12.6399109321793279   T   T   T
  6.8658172692477359  7.2159543023887878 12.8778230036465562   T   T   T
 10.7645356309395002  9.8280576332175897 12.8775860971143086   T   T   T
  9.7951794426905394 10.4529195223421922  7.9999999999999991   F   F   F
  7.8361721654953271 13.0649280100698402  8.0000055199296654   F   F   F
  9.7951793303235473 12.4334987916241673  8.0000008619369254   F   F   F
  7.8361729104275160 15.0455072824293214  8.0000049280612373   F   F   F
  6.8566642656580949 10.4529195414531415  9.6370125635575050   F   F   F
 10.7746760734116016 13.0649280291807894  9.6370180834871739   F   F   F
  6.8566641532911001 12.4334988107351183  9.6370134254944340   F   F   F
 10.7746768183437940 15.0455073015402707  9.6370174916187459   F   F   F
  9.7426031147532601 10.4396774678586581 11.3119181410270624   T   T   T
  7.8864858938636138 13.0531820991758707 11.3119624746994329   T   T   T
  9.7853303861509495 12.4422264867355050 11.2951978897793719   T   T   T
  7.8445614928307066 15.0545716373972187 11.2956021961770077   T   T   T
  6.6154043752272811 10.5814914039206922 12.6360897630835076   T   T   T
 11.0116511677106015 13.1918639793725756 12.6395973879100456   T   T   T
  6.8642554300842908 12.4408526068453984 12.8770285328031004   T   T   T
 10.7653035505176575 15.0518757886680792 12.8777395377616575   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Pt E_tot= -429.86626798
eV
 D3-zero damping= -33.0741974 eV, D3-BJ damping= -34.6536169 eV
Pt
 1.0000000000000000
    11.7540381698974450    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.6720508931965945    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.8624102375939486
  72
Cartesian
 -0.0000000761175146  1.9590065626350686  7.9940155928349457
  1.9590063331035370 -0.0000000295699861  7.9940157360039441
  0.0000000708635028 -0.0000001612413123  9.9312051349566453
  1.9590065446590228  1.9590062109948447  9.9312049159985332
 -0.0000000549863877  1.9590063833668176 11.8683948277430478
  1.9590063473892791 -0.0000000401145291 11.8683946994723684
 -0.0000001972697436  5.8770189278189484  7.9940157254661051
  1.9590063759353173  3.9180127703099572  7.9940155350794386
```

-0.0000000253909557	3.9180128560198684	9.9312049414347694
1.9590063293623401	5.8770189806300657	9.9312052580758881
0.0000000180014927	5.8770190309442443	11.8683945121278729
1.9590063473638331	3.9180128612993301	11.8683946701951974
0.0000000872736213	9.7950317178191781	7.9940152761937933
1.9590063939368101	7.8360254195905137	7.9940155281963232
0.0000000105445430	7.8360249356021452	9.9312048002819253
1.9590065446335767	9.7950316538265003	9.9312051021177510
0.0000001084047481	9.7950317299948981	11.8683948475277052
1.9590065806365622	7.8360254465982973	11.8683945955251762
0.0000000111306608	13.7130445458327532	7.9940157104552663
1.9590063901956134	11.7540382873084770	7.9940155237233874
0.0000003422215542	11.7540384544408045	9.9312051567380699
1.9590062632286978	13.7130448980845507	9.9312051672759374
0.0000001686982620	13.7130445278312632	11.8683946485068859
1.9590064557685836	11.7540380577515062	11.8683947393068365
3.9180127851563702	1.9590064262240412	7.9940155393468624
5.8770189781076825	0.0000000185621647	7.9940157509022782
3.9180127090134080	0.0000003317190521	9.9312049445699788
5.8770190357858647	1.9590064014192050	9.9312048183155071
3.9180127528691351	1.9590063722361568	11.8683945880294583
5.8770191468059414	-0.0000000105699889	11.8683946883218674
3.9180127090134080	5.8770191573759343	7.9940156420688364
5.8770189601061906	3.9180128010080346	7.9940157509023422
3.9180126910119153	3.9180126730104203	9.9312051101330159
5.8770190960793833	5.8770187178128026	9.9312051529902234
3.9180126941669964	5.8770191250886921	11.8683947236833536
5.8770190812329659	3.9180127740257076	11.8683947056497789
3.9180127270149008	9.7950318119381823	7.9940154951519027
5.8770190637921553	7.8360253583194188	7.9940154739831497
3.9180124281946473	7.8360251471576250	9.9312050486295949
5.8770187935599756	9.7950316749576221	9.9312049864011680
3.9180126434404379	9.7950319098238321	11.8683946502579882
5.8770190526614936	7.8360252673046009	11.8683947074939162
3.9180127375848928	13.7130446204120222	7.9940156052765445
5.8770190373772397	11.7540381338944595	7.9940153906788378
3.9180125931683065	11.7540381984523314	9.9312051281665976
5.8770192573627380	13.7130448378164900	9.9312051815617206
3.9180125403151491	13.7130444337122572	11.8683947505503458
5.8770190342476081	11.7540381518959531	11.8683948475277319
7.8360252381724464	1.9590065626350686	7.9940156761391910
9.7950318262493639	0.0000000179760469	7.9940156176585591
7.8360252636142880	0.0000001878510739	9.9312050920994377
9.7950316289796202	1.9590065843777580	9.9312051063851960
7.8360254323125593	1.9590063653653249	11.8683947730102872
9.7950318405350991	-0.0000000904287013	11.8683946125327573
7.8360254608840316	5.8770190780778915	7.9940155536325985
9.7950318119636286	3.9180128914367383	7.9940156401650766
7.8360254608585862	3.9180126761909482	9.9312050778136776
9.7950317865472307	5.8770188156730079	9.9312051641407280
7.8360255227412505	5.8770190346600009	11.8683947019949656
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7.8360254788855244	13.7130445241155066	11.8683945632058805

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  9.7950318225336073 11.7540382603261371 11.8683951206990272

Interface: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Pd E_tot= -804.53696895 eV
 D3-zero damping= -49.677662 eV, D3-BJ damping= -53.4929559 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Pd
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     0.0000000000000000   15.5449293091988210    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.9240623731285034
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2  72
Selective dynamics
Cartesian
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  3.8863783198123127  1.9693600505045268  8.0000008619369254   F   F   F
  1.9432620983884621  4.5601816105735837  8.0000049280612373   F   F   F
  0.9716985969389017  0.0048459837119056  9.6370125635575068   F   F   F
  4.8579300161192815  2.5956675407284169  9.6370180834871757   F   F   F
  0.9716984854833554  1.9693600694604616  9.6370134254944340   F   F   F
  4.8579307550090620  4.5601816295295174  9.6370174916187459   F   F   F
  3.9238085417255140  0.0103923123408519 11.3654656890781798   T   T   T
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  0.9140056499306903 -0.1246976157004774 12.8628776412838928   T   T   T
  4.8925711431119225  2.5771277968179249 12.9123796511262778   T   T   T
  0.7208552016009275  1.8528687269843744 12.7381474746171701   T   T   T
  4.7965586027965221  4.6199255363236045 12.8948745960731657   T   T   T
  3.8863785977473557  5.1864890678222411  8.0000000000000000   F   F   F
  1.9432615259781783  7.7773106248387531  8.0000055199296671   F   F   F
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  4.8579301825987793  7.7773106437946895  9.6370180834871757   F   F   F
  0.9716986519628530  7.1510031725267336  9.6370134254944340   F   F   F
  4.8579309214885606  9.7418247325957879  9.6370174916187459   F   F   F
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  3.8217602844526195  7.1080437929224773 11.2071049766325554   T   T   T
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Oxide reference: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Pd E_tot= -417.94525959
eV
 D3-zero damping= -12.6525572 eV, D3-BJ damping= -14.2514383 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
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2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.8863784312678584  0.0048459647559709  7.9999999999999991   F   F   F
  1.9432613594986810  2.5956675217724823  8.0000055199296654   F   F   F
  3.8863783198123127  1.9693600505045268  8.0000008619369254   F   F   F
  1.9432620983884621  4.5601816105735837  8.0000049280612373   F   F   F
  0.9716985969389017  0.0048459837119056  9.6370125635575050   F   F   F
  4.8579300161192815  2.5956675407284169  9.6370180834871739   F   F   F
  0.9716984854833554  1.9693600694604616  9.6370134254944340   F   F   F
  4.8579307550090620  4.5601816295295174  9.6370174916187459   F   F   F
  3.8410917068365484 -0.0188746653433774 11.3204847512649014   T   T   T
  1.9886268767812012  2.5715300805605050 11.3205700995947804   T   T   T
  3.8876347198171244  1.9789151726083059 11.3025404429588860   T   T   T
  1.9434665170365830  4.5691348095358446 11.3022708073571074   T   T   T
  0.7426582382357280  0.1216042176894928 12.6764495999603124   T   T   T
  5.0914209731749080  2.7115652687270444 12.6734211943982373   T   T   T
  0.9989060152401599  1.9803212901193485 12.9140338969241952   T   T   T
  4.8348094150765615  4.5704945048139098 12.9132852396082054   T   T   T
  3.8863785977473557  5.1864890678222411  7.9999999999999991   F   F   F
  1.9432615259781783  7.7773106248387531  8.0000055199296654   F   F   F
  3.8863784862918100  7.1510031535707990  8.0000008619369254   F   F   F
  1.9432622648679601  9.7418247136398559  8.0000049280612373   F   F   F
  0.9716987634183991  5.1864890867781774  9.6370125635575050   F   F   F
  4.8579301825987793  7.7773106437946895  9.6370180834871739   F   F   F
  0.9716986519628530  7.1510031725267336  9.6370134254944340   F   F   F
  4.8579309214885606  9.7418247325957879  9.6370174916187459   F   F   F
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  1.9883657414633737  7.7535094990453537 11.3205612927588870   T   T   T
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  0.7433421588739009  5.3020278158790024 12.6754927344777109   T   T   T
  5.0867757274730936  7.8941104655826306 12.6765413553809747   T   T   T
  0.9956730311864025  7.1618995522021214 12.9124498119194744   T   T   T
  4.8305114208976283  9.7528096412854914 12.9140144291938608   T   T   T
  3.8863787642268535 10.3681321708885132  7.9999999999999991   F   F   F
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  1.9432624313474574 14.9234678167061254  8.0000049280612373   F   F   F
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  4.8579303490782770 12.9589537468609599  9.6370180834871739   F   F   F
  0.9716988184423505 12.3326462755930066  9.6370134254944340   F   F   F
  4.8579310879680575 14.9234678356620609  9.6370174916187459   F   F   F
  3.8408736498183123 10.3440019802392964 11.3204939126651976   T   T   T
  1.9869116907667379 12.9354489738532266 11.3219167472878155   T   T   T
  3.8859904166533674 12.3415976861106262 11.3022139840425417   T   T   T
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  4.8337477829202671 14.9343474967776721 12.9123344692684086   T   T   T
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  7.7726105893380186  4.5601816105735837  8.0000049280612373   F   F   F
  6.8010470878884570  0.0048459837119056  9.6370125635575050   F   F   F
 10.6872785070688412  2.5956675407284169  9.6370180834871739   F   F   F
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  9.6704401118847496 -0.0188746446235235 11.3204847588510056   T   T   T
  7.8179753516565302  2.5715302432211096 11.3205700057570517   T   T   T
  9.7169831766930503  1.9789151945051544 11.3025404494001336   T   T   T
  7.7728148968676223  4.5691349245934987 11.3022709033171527   T   T   T
  6.5720067515460530  0.1216040020639810 12.6764495442523444   T   T   T
 10.9207693439052012  2.7115652820780469 12.6734212707979417   T   T   T
  6.8282545843659710  1.9803211513307195 12.9140337564947920   T   T   T
 10.6641579121523034  4.5704945407536961 12.9132853262210237   T   T   T
  9.7157270886969123  5.1864890678222411  7.9999999999999991   F   F   F
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  6.8010472543679557  5.1864890867781774  9.6370125635575050   F   F   F
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  6.8010471429124113  7.1510031725267336  9.6370134254944340   F   F   F
 10.6872794124381159  9.7418247325957879  9.6370174916187459   F   F   F
  9.6718818206159494  5.1629615547868362 11.3218826325821151   T   T   T
  7.8177143109229137  7.7535094982776807 11.3205613095489444   T   T   T
  9.7161015118585610  7.1598057721428772 11.3029334900654739   T   T   T
  7.7712252748136281  9.7513529652564781 11.3025488784443731   T   T   T
  6.5726905486153031  5.3020281908183700 12.6754926939456816   T   T   T
 10.9161242977545854  7.8941103244472970 12.6765414466730686   T   T   T
  6.8250214963173237  7.1618996914213762 12.9124498225836621   T   T   T
 10.6598599512388930  9.7528095835228843 12.9140146583562174   T   T   T
  9.7157272551764091 10.3681321708885132  7.9999999999999991   F   F   F
  7.7726101834072345 12.9589537279050244  8.0000055199296654   F   F   F
  9.7157271437208657 12.3326462566370711  8.0000008619369254   F   F   F
  7.7726109222970141 14.9234678167061254  8.0000049280612373   F   F   F
  6.8010474208474534 10.3681321898444487  9.6370125635575050   F   F   F
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  6.8010473093919082 12.3326462755930066  9.6370134254944340   F   F   F
 10.6872795789176163 14.9234678356620609  9.6370174916187459   F   F   F
  9.6702222160653601 10.3440019039650899 11.3204940920028267   T   T   T
  7.8162602098521026 12.9354488162228449 11.3219168755611310   T   T   T
  9.7153390188545750 12.3415976148927005 11.3022140198219248   T   T   T
  7.7720743760074962 14.9322729882226994 11.3029259121375709   T   T   T
  6.5673358700995559 10.4840432375089403 12.6733127445887988   T   T   T
 10.9153169570024353 13.0744556174693773 12.6754860404911636   T   T   T
  6.8239122350737613 12.3429813773941568 12.9132852862719858   T   T   T
 10.6630962783245931 14.9343474580674886 12.9123344286672079   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Pd E_tot= -365.30961581
eV
 D3-zero damping= -24.4487943 eV, D3-BJ damping= -29.8711642 eV
Pd
 1.0000000000000000
    11.6586969818991157    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.5449293091988210    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.8984851893707742
  72
Cartesian
  0.0000000142602950  1.9431161493641240  7.9925930295093428
  1.9431161636498535  0.0000000072690022  7.9925932083064248
  0.0000002505038900  0.0000000000000000  9.9492425729786156
  1.9431164284394722  1.9431161636498526  9.9492428091967842
  0.0000000000000000  1.9431161278602589 11.9058921671433673
  1.9431161636498535 -0.0000000000000000 11.9058921534901287
  0.0000000142602950  5.8293484909495579  7.9925930149454487
  1.9431161564062849  3.8862323200307043  7.9925928282339029
  0.0000002505038900  3.8862323272997052  9.9492425586928945
  1.9431161636498535  5.8293485124788553  9.9492425875425212
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0.0000000215292972	5.8293484909495579	11.9058921240080196
1.9431161636498535	3.8862323488035702	11.9058921240080196
-0.0000000215292972	9.7155807967199657	7.9925930787377828
1.9431161636498535	7.7724646618684190	7.9925929790920405
-0.0000000142602950	7.7724646904144290	9.9492425945462877
1.9431161493895568	9.7155808182492613	9.9492425802605666
-0.0000000142602950	9.7155808325095521	11.9058923180015235
1.9431161636498535	7.7724646473558350	11.9058921030728158
-0.0000000358150241	13.6018131813639869	7.9925932441598366
1.9431161636498535	11.6586969961594047	7.9925930644520724
-0.0000000142602950	11.6586969460840972	9.9492423297566770
1.9431161636498535	13.6018131455235363	9.9492425875425319
-0.0000000000000000	13.6018131455489684	11.9058921741471160
1.9431161636498535	11.6586970034284132	11.9058921024403368
3.8862323130394110	1.9431161278348268	7.9925930501663363
5.8293484766638368	0.0000000215547290	7.9925929505205984
3.8862323272997070	0.0000000358150241	9.9492426018282423
5.8293482261599472	1.9431161636752845	9.9492425945462770
3.8862323272997070	1.9431161278602589	11.9058921319224567
5.8293484766892680	0.0000002505038900	11.9058921677758818
3.8862323130394110	5.8293485124788553	7.9925932295959567
5.8293484909495579	3.8862323057449757	7.9925930006597419
3.8862323272997070	3.8862320625100866	9.9492425875425212
5.8293484909495579	5.8293484766638368	9.9492423513243526
3.8862320767958169	5.8293484909495579	11.9058921094441370
5.8293484909495579	3.8862323345432741	11.9058920745013896
3.8862323272997070	9.7155807824596749	7.9925930644520857
5.8293485124788553	7.7724644755145169	7.9925929863740057
3.8862323272997070	7.7724646904144290	9.9492426018282423
5.8293484909495579	9.7155808182492613	9.9492425945462770
3.8862323272997070	9.7155808325095521	11.9058920745013754
5.8293484909495579	7.7724646972201024	11.9058921525794403
3.8862323272997070	13.6018131813639869	7.9925932584455577
5.8293485124788553	11.6586969961594047	7.9925931003054691
3.8862323415854356	11.6586969460840972	9.9492423297566770
5.8293484909495579	13.6018130455839632	9.9492423513243526
3.8862323272997070	13.6018131813639869	11.9058921884328672
5.8293484909495579	11.6586969818991157	11.9058923107195582
7.7724646545994087	1.9431161493641240	7.9925929936559568
9.7155808182492631	-0.0000000568809923	7.9925929578025636
7.7724646545994087	0.0000000142857269	9.9492425945462877
9.7155808325095538	1.9431161779355812	9.9492428019148189
7.7724646545994087	1.9431161278602589	11.9058921671433673
9.7155808182492631	-0.0000000000000000	11.9058922315682256
7.7724646545994087	5.8293484909495579	7.9925930006597419
9.7155808182492631	3.8862323200307043	7.9925930437950603
7.7724646545994087	3.8862323272997052	9.9492425802605666
9.7155808182492631	5.8293485052098468	9.9492425802605666
7.7724646545994087	5.8293485052098468	11.9058921525794403
9.7155808182492631	3.8862323488290027	11.9058921455756845
7.7724646545994087	9.7155807967199657	7.9925928355158682
9.7155808325095538	7.7724647402786964	7.9925930222273882
7.7724646688596986	7.7724646904144290	9.9492425586928945
9.7155808325095538	9.7155808182492613	9.9492425729786014
7.7724646688596986	9.7155808182492613	11.9058920960690617
9.7155808182492631	7.7724647114803913	11.9058921176367463
7.7724646904144272	13.6018131172140002	7.9925932584455577
9.7155808325095538	11.6586970104451257	7.9925931003054549
7.7724646688596986	11.6586969460840972	9.9492423297566770
9.7155808325095538	13.6018131312632473	9.9492422516786263
7.7724646545994087	13.6018131670782658	11.9058922027185741
9.7155808182492631	11.6586967171349372	11.9058923250052793

```
Interface: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Ir E_tot= -1046.3690673 eV
 D3-zero damping= -55.571367 eV, D3-BJ damping= -56.9268628 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Ir
 1.0000000000000000
    11.5190376621507102    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.3587168828676166    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.7441275142506072
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2  72
Selective dynamics
Cartesian
  3.8398235745082716  0.0047879150320271  8.0000000000000000   F   F   F
  1.9199830669088396  2.5645740675943189  8.0000055199296671   F   F   F
  3.8398234643878499  1.9457691221683533  8.0000008619369254   F   F   F
  1.9199837969474736  4.5055552777466250  8.0000049280612373   F   F   F
  0.9600586370651988  0.0047879337608890  9.6370125635575068   F   F   F
  4.7997369605411215  2.5645740863231810  9.6370180834871757   F   F   F
  0.9600585269447764  1.9457691408972153  9.6370134254944340   F   F   F
  4.7997376905797555  4.5055552964754852  9.6370174916187459   F   F   F
  3.8936791751988244  0.0059314021578225 11.3830921063595483   T   T   T
  1.8407757489696566  2.4403295405545942 11.4417231223666231   T   T   T
  3.8099625499951060  2.0140536471228128 11.3213020298733458   T   T   T
  1.8799968880527693  4.4330506423599960 11.2922364619096811   T   T   T
  0.8979155429992198 -0.2080349967690568 12.9073138001148937   T   T   T
  4.8491206304552321  2.3797129965821888 12.9308173736252119   T   T   T
  0.5399721891606758  1.7934315585784550 12.7999421799615121   T   T   T
  4.7164502682060148  4.6955247117252679 13.1081681922186206   T   T   T
  3.8398237389935139  5.1243602093212290  8.0000000000000000   F   F   F
  1.9199832313940821  7.6841463618835215  8.0000055199296671   F   F   F
  3.8398236288730923  7.0653414164575565  8.0000008619369254   F   F   F
  1.9199839614327165  9.6251275720358276  8.0000049280612373   F   F   F
  0.9600588015504413  5.1243602280500919  9.6370125635575068   F   F   F
  4.7997371250263647  7.6841463806123844  9.6370180834871757   F   F   F
  0.9600586914300192  7.0653414351864194  9.6370134254944340   F   F   F
  4.7997378550649987  9.6251275907646878  9.6370174916187459   F   F   F
  3.7833934918542407  4.9971462754373208 11.3159260963764368   T   T   T
  1.9446946591246568  7.6149773960334262 11.2246384067460436   T   T   T
  3.7929634545854336  6.9746630104667080 11.2152761356079829   T   T   T
  2.0359988946527268  9.5863765219558399 11.1694710826831063   T   T   T
  0.9681529728867694  4.8532783532377843 12.9501889978135640   T   T   T
  4.2350044634102550  7.6164886494398036 12.9907926849754123   T   T   T
  1.0791188803391414  6.9696180169096777 12.8710094739380008   T   T   T
  4.6859714234942995  9.6414508036128161 12.8167482564983235   T   T   T
  3.8398239034787567 10.2439325036104343  8.0000000000000000   F   F   F
  1.9199833958793251 12.8037186561727250  8.0000055199296671   F   F   F
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  1.9199841259179591 14.7446998663250284  8.0000049280612373   F   F   F
  0.9600589660356839 10.2439325223392945  9.6370125635575068   F   F   F
  4.7997372895116079 12.8037186749015852  9.6370180834871757   F   F   F
  0.9600588559152619 12.1849137294756229  9.6370134254944340   F   F   F
  4.7997380195502410 14.7446998850538904  9.6370174916187459   F   F   F
  3.8475837844311878 10.3222118376494851 11.2125121898027125   T   T   T
  1.9644056895837021 12.7834224217823742 11.3126558633625454   T   T   T
  3.8993147417421161 12.2844732239302683 11.3196523088910954   T   T   T
  1.9725919768989928 14.7705970274924585 11.2969273030712980   T   T   T
  1.4421000188255131  9.9605733647928432 12.9583510970551217   T   T   T
  4.8262221215012318 12.9447011454965892 12.9000662601800311   T   T   T
  1.0960924077228087 12.0195275131175343 12.8923239184721030   T   T   T
  5.2098520786018359 14.9364666326560176 12.8252905744913175   T   T   T
  9.5993424055836272  0.0047879150320271  8.0000000000000000   F   F   F
  7.6795018979841956  2.5645740675943189  8.0000055199296671   F   F   F
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9.5993422954632059	1.9457691221683533	8.0000008619369254	F	F	F
7.6795026280228269	4.5055552777466250	8.0000049280612373	F	F	F
6.7195774681405522	0.0047879337608890	9.6370125635575068	F	F	F
10.5592557916164775	2.5645740863231810	9.6370180834871757	F	F	F
6.7195773580201310	1.9457691408972153	9.6370134254944340	F	F	F
10.5592565216551098	4.5055552964754852	9.6370174916187459	F	F	F
9.5745947866146626	-0.0643510218580181	11.2246427721670177	T	T	T
7.6717265622998028	2.6429286679430399	11.2124869684192188	T	T	T
9.4832280425024305	1.9070237807665911	11.1694127072539260	T	T	T
7.6200033734629269	4.6051664218048760	11.3196929690885550	T	T	T
7.2842754335534670	-0.0626893666175580	12.9909002708376384	T	T	T
10.0770160092425041	2.2811522719658655	12.9583354412575744	T	T	T
6.8331778625881405	1.9622045957439183	12.8166978627700470	T	T	T
10.4229887971498076	4.3400806933321903	12.8923433141951254	T	T	T
9.5993425700688704	5.1243602093212290	8.0000000000000000	F	F	F
7.6795020624694388	7.6841463618835215	8.0000055199296671	F	F	F
9.5993424599484474	7.0653414164575565	8.0000008619369254	F	F	F
7.6795027925080701	9.6251275720358276	8.0000049280612373	F	F	F
6.7195776326257954	5.1243602280500919	9.6370125635575068	F	F	F
10.5592559561017190	7.6841463806123844	9.6370180834871757	F	F	F
6.7195775225053742	7.0653414351864194	9.6370134254944340	F	F	F
10.5592566861403530	9.6251275907646878	9.6370174916187459	F	F	F
9.5549087905326058	5.1041360159143903	11.3126403874076757	T	T	T
7.6255767069876965	7.6852428337538816	11.3831492964101901	T	T	T
9.5466772370386490	7.0912793753258132	11.2968960696751815	T	T	T
7.7092661312663813	9.6933427972192092	11.3212874493925426	T	T	T
6.6929209171528861	5.2652646383907618	12.9000491646589630	T	T	T
10.6212883127551798	7.4713220304603967	12.9073617661896769	T	T	T
6.3093654345362609	7.2570551838422963	12.8252956832907294	T	T	T
10.9791532152466917	9.4727904099016769	12.7999688468683690	T	T	T
9.5993427345541118	10.2439325036104343	8.0000000000000000	F	F	F
7.6795022269546820	12.8037186561727250	8.0000055199296671	F	F	F
9.5993426244336906	12.1849137107467609	8.0000008619369254	F	F	F
7.6795029569933133	14.7446998663250284	8.0000049280612373	F	F	F
6.7195777971110386	10.2439325223392945	9.6370125635575068	F	F	F
10.5592561205869622	12.8037186749015852	9.6370180834871757	F	F	F
6.7195776869906165	12.1849137294756229	9.6370134254944340	F	F	F
10.5592568506255962	14.7446998850538904	9.6370174916187459	F	F	F
9.6783716375282562	10.1195874740165248	11.4416787651282732	T	T	T
7.7357698244463027	12.6767031396430525	11.3159349840061072	T	T	T
9.6392000441991179	12.1124028841568396	11.2921715172343333	T	T	T
7.7262726272326550	14.6541608417123435	11.2153431192330686	T	T	T
6.6700968975580119	10.0590861399213072	12.9307445302026736	T	T	T
10.5508379978848268	12.5325581278970688	12.9502024110543807	T	T	T
6.8026639735681735	12.3748690303517108	13.1080951058815476	T	T	T
10.4400397834125513	14.6489228839404788	12.8710950422631480	T	T	T
0.1588627023065219	1.8922111180762264	14.9255670264809570	T	T	T
1.9755763619193225	-0.0296323486595953	15.1403850002622402	T	T	T
-0.0289977562089585	0.0261567658461995	16.8657219203339146	T	T	T
1.9017478978937634	1.9124631077285676	16.9633340032336477	T	T	T
-0.0548342273770862	1.9108219310273467	18.7243671737838220	T	T	T
1.8773839325822423	-0.0306523268777325	18.7581831291777270	T	T	T
-0.0492295697330105	5.7773850432441254	15.1021392123445928	T	T	T
1.9491535278788423	3.8057908412465036	15.0534654633359164	T	T	T
-0.0048083253554234	3.7967191847084480	16.8516235418828408	T	T	T
1.9569540531746965	5.7782081800559828	16.7880010850756278	T	T	T
0.0601781657390167	5.7518429049682220	18.7159264278639625	T	T	T
1.9140628878641972	3.8894907325690697	18.7081138406738177	T	T	T
-0.1589041211954502	9.5715862229137532	14.9255412640254779	T	T	T
1.9124209015259650	7.6448618116238709	14.7622121399694421	T	T	T
0.0289084407327489	7.7055373833076670	16.8656867271138573	T	T	T
1.9174318544494255	9.5751908459103241	16.6580026751808674	T	T	T
0.0547330551551212	9.5901664898547807	18.7243632186046582	T	T	T

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  1.9706507983013075  7.6918274198225953 18.6241041011207571   T   T   T
  0.0491641585970217 13.4567455688951654 15.1021453976431008   T   T   T
  1.9141872636443535 11.6183081612335979 14.8769235866256455   T   T   T
  0.0047245642386307 11.4760985667599300 16.8516263559036759   T   T   T
  1.9032272526097456 13.3929257116511593 16.9679255266898004   T   T   T
 -0.0602807754478537 13.4312059530819834 18.7159443131005361   T   T   T
  1.9330940757702542 11.4271091371364619 18.6885157346648398   T   T   T
  3.7677797810042311  1.8908622057459594 15.1027291120373501   T   T   T
  5.5894019938638522 -0.0313689359082794 14.9271696049936491   T   T   T
  3.8584258390714359 -0.0186639166717651 16.9838414254924643   T   T   T
  5.7788767270898589  1.8862441008638786 16.8052114167138384   T   T   T
  3.8848368829859603  1.9434888507645254 18.7414468857083918   T   T   T
  5.8312376047168470 -0.0005401725104331 18.6994829709080257   T   T   T
  3.8246091614761499  5.6894116110707778 14.8463588250833141   T   T   T
  5.7606465746072244  3.8261939015290620 14.9956657471529731   T   T   T
  3.8573767655028544  3.8417034969173147 16.8965054829570178   T   T   T
  5.7624981610820161  5.7578239309069446 16.8598034494522970   T   T   T
  3.8322450722032921  5.8042169181782093 18.6697343424737738   T   T   T
  5.7918608142998682  3.8116054538286757 18.6969981010784103   T   T   T
  3.8572374185288876  9.6539572937243623 14.7930403129023613   T   T   T
  5.9295645114102982  7.6479919900742530 14.9272007570373155   T   T   T
  3.8443643502488145  7.6732376576897829 16.6540448357760020   T   T   T
  5.7400766066959550  9.5656105836742640 16.8052360102033447   T   T   T
  3.8127335290440891  9.5552915118765025 18.6225182112079501   T   T   T
  5.6877205692955952  7.6788100016837122 18.6994993708705231   T   T   T
  3.7704201755567381 13.4467805603794499 15.1042221740673668   T   T   T
  5.7583237239212384 11.5055289006817016 14.9956481775363937   T   T   T
  3.8173373413283764 11.4628707047985525 16.7868641283896025   T   T   T
  5.7564515574269777 13.4371770606424423 16.8597547272913175   T   T   T
  3.8647250672370501 13.3644074362647949 18.7310540157426964   T   T   T
  5.7270802706954340 11.4909661633138995 18.6969832489574408   T   T   T
  7.6617429759904798  1.9746256431380078 14.7930636856293507   T   T   T
  9.6065596953865260 -0.0344783650731080 14.7621846861138835   T   T   T
  7.6745945925546337 -0.0061173240057621 16.6540376328413835   T   T   T
  9.6015367154867217  1.8958321325635661 16.6579930550061768   T   T   T
  7.7062119379816423  1.8759411646436741 18.6225080540166346   T   T   T
  9.5482730781752228  0.0125019813387367 18.6241220505787091   T   T   T
  7.7485384053766042  5.7674206334442299 15.1042484008319189   T   T   T
  9.6047869462612869  3.9389241051163091 14.8769089352067780   T   T   T
  7.7016211958568723  3.7835160065232305 16.7868715575419252   T   T   T
  9.6157343144483676  5.7135758127820218 16.9679107460267815   T   T   T
  7.6542426853554524  5.6850515014105607 18.7310675122412249   T   T   T
  9.5858436856366644  3.7477726585048745 18.6884970421322301   T   T   T
  7.7511753937922734  9.5702110998279224 15.1027469600356046   T   T   T
  9.5433705757927587  7.6497359747698299 15.1403324264896089   T   T   T
  7.6605483383168593  7.6607009625287725 16.9838567843172754   T   T   T
  9.6172099154281252  9.5918102946790178 16.9633277706765817   T   T   T
  7.6341188644299631  9.6228591635687728 18.7414538532716044   T   T   T
  9.6415693375765059  7.6487056340779516 18.7581758250846491   T   T   T
  7.6943619976485831 13.3687500119566636 14.8463712927811446   T   T   T
  9.5697969334731958 11.4851492529027919 15.0534839635671407   T   T   T
  7.6615608539801716 11.5210586813655986 16.8964944625543616   T   T   T
  9.5619971216563044 13.4575590296356022 16.7880260286995586   T   T   T
  7.6867002908634081 13.4835748995656299 18.6697224140164479   T   T   T
  9.6048549889715993 11.5688292472250538 18.7081166383307576   T   T   T

Oxide reference: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Ir E_tot= -418.15122055
eV
 D3-zero damping= -12.8031107 eV, D3-BJ damping= -14.520941 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
    11.5190376621507102    0.0000000000000000    0.0000000000000000
```

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     0.0000000000000000   15.3587168828676166    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.9609982221306907
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.8398235745082716  0.0047879150320271  8.0000000000000000   F   F   F
  1.9199830669088396  2.5645740675943189  8.0000055199296689   F   F   F
  3.8398234643878499  1.9457691221683533  8.0000008619369254   F   F   F
  1.9199837969474736  4.5055552777466250  8.0000049280612373   F   F   F
  0.9600586370651988  0.0047879337608890  9.6370125635575086   F   F   F
  4.7997369605411215  2.5645740863231810  9.6370180834871775   F   F   F
  0.9600585269447764  1.9457691408972153  9.6370134254944340   F   F   F
  4.7997376905797555  4.5055552964754852  9.6370174916187459   F   F   F
  3.8075102413144681 -0.0333016894035915 11.3346210533890659   T   T   T
  1.9523648488690597  2.5227159404608646 11.3345926391886280   T   T   T
  3.8540135305483574  1.9580815805433163 11.3138198244442627   T   T   T
  1.9053665496272696  4.5147918208103848 11.3133210709780396   T   T   T
  0.7451364165142923  0.1013349478782917 12.7289417388302439   T   T   T
  5.0166306593311090  2.6641150605313673 12.7301652746491545   T   T   T
  1.0073765102962815  1.9606887953692766 12.9661310992651142   T   T   T
  4.7510908244005776  4.5223242604378253 12.9668711547147755   T   T   T
  3.8398237389935139  5.1243602093212290  8.0000000000000000   F   F   F
  1.9199832313940821  7.6841463618835215  8.0000055199296689   F   F   F
  3.8398236288730923  7.0653414164575565  8.0000008619369254   F   F   F
  1.9199839614327165  9.6251275720358276  8.0000049280612373   F   F   F
  0.9600588015504413  5.1243602280500919  9.6370125635575086   F   F   F
  4.7997371250263647  7.6841463806123844  9.6370180834871775   F   F   F
  0.9600586914300192  7.0653414351864194  9.6370134254944340   F   F   F
  4.7997378550649987  9.6251275907646878  9.6370174916187459   F   F   F
  3.8056159500420996  5.0834859552969194 11.3350998877144509   T   T   T
  1.9522976901582423  7.6460783603538873 11.3346122510520448   T   T   T
  3.8523989244445525  7.0752603596913577 11.3128691066360876   T   T   T
  1.9056857734095296  9.6373924517110847 11.3138265331518131   T   T   T
  0.7432017714129715  5.2224854178590361 12.7279872043778255   T   T   T
  5.0146407459480464  7.7807423074687705 12.7287862240776448   T   T   T
  1.0072054361216887  7.0810260587504752 12.9651806480120939   T   T   T
  4.7521909396479174  9.6400682882099975 12.9661354043377557   T   T   T
  3.8398239034787567 10.2439325036104343  8.0000000000000000   F   F   F
  1.9199833958793251 12.8037186561727250  8.0000055199296689   F   F   F
  3.8398237933583355 12.1849137107467609  8.0000008619369254   F   F   F
  1.9199841259179591 14.7446998663250284  8.0000049280612373   F   F   F
  0.9600589660356839 10.2439325223392945  9.6370125635575086   F   F   F
  4.7997372895116079 12.8037186749015852  9.6370180834871775   F   F   F
  0.9600588559152619 12.1849137294756229  9.6370134254944340   F   F   F
  4.7997380195502410 14.7446998850538904  9.6370174916187459   F   F   F
  3.8072764281638851 10.2020790109241499 11.3345026282943593   T   T   T
  1.9541450245443968 12.7628530591515066 11.3351244654337293   T   T   T
  3.8543615145985295 12.1941200791696716 11.3132562866068387   T   T   T
  1.9073503569456538 14.7546554915730788 11.3129069695011797   T   T   T
  0.7431053150935543 10.3434200806328960 12.7302157357482848   T   T   T
  5.0165216372656030 12.9017580234691600 12.7279492064913278   T   T   T
  1.0085599647742882 12.2015567354581940 12.9667951161522943   T   T   T
  4.7525327011446281 14.7603299585509813 12.9652133226929376   T   T   T
  9.5993424055836272  0.0047879150320271  8.0000000000000000   F   F   F
  7.6795018979841956  2.5645740675943189  8.0000055199296689   F   F   F
  9.5993422954632059  1.9457691221683533  8.0000008619369254   F   F   F
  7.6795026280228269  4.5055552777466250  8.0000049280612373   F   F   F
  6.7195774681405522  0.0047879337608890  9.6370125635575086   F   F   F
 10.5592557916164775  2.5645740863231810  9.6370180834871775   F   F   F
  6.7195773580201310  1.9457691408972153  9.6370134254944340   F   F   F
 10.5592565216551098  4.5055552964754852  9.6370174916187459   F   F   F
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  9.5670290710892409 -0.0333015981902593 11.3346209109329816   T   T   T
  7.7118837897306465  2.5227158366410731 11.3345925868754289   T   T   T
  9.6135323434614008  1.9580816636318519 11.3138199377919424   T   T   T
  7.6648853178622902  4.5147918059980485 11.3133211060250787   T   T   T
  6.5046554260702250  0.1013347550753669 12.7289418155090779   T   T   T
 10.7761493869009293  2.6641152547957443 12.7301654468661081   T   T   T
  6.7668954261660810  1.9606886672115307 12.9661309827711477   T   T   T
 10.5106094780377148  4.5223244101205982 12.9668711562804084   T   T   T
  9.5993425700688704  5.1243602093212290  8.0000000000000000   F   F   F
  7.6795020624694388  7.6841463618835215  8.0000055199296689   F   F   F
  9.5993424599484474  7.0653414164575565  8.0000008619369254   F   F   F
  7.6795027925080701  9.6251275720358276  8.0000049280612373   F   F   F
  6.7195776326257954  5.1243602280500919  9.6370125635575086   F   F   F
 10.5592559561017190  7.6841463806123844  9.6370180834871775   F   F   F
  6.7195775225053742  7.0653414351864194  9.6370134254944340   F   F   F
 10.5592566861403530  9.6251275907646878  9.6370174916187459   F   F   F
  9.5651348121083881  5.0834859530291556 11.3350998048431428   T   T   T
  7.7118163924133496  7.6460783986507481 11.3346122113574896   T   T   T
  9.6119178825210039  7.0752604602287130 11.3128690616934851   T   T   T
  7.6652046576256465  9.6373925120918162 11.3138264857950137   T   T   T
  6.5027207195814380  5.2224853092918515 12.7279869865582000   T   T   T
 10.7741595284142697  7.7807422835699684 12.7287861584309017   T   T   T
  6.7667243634047560  7.0810258960911447 12.9651806376353687   T   T   T
 10.5117097158607695  9.6400682468435317 12.9661353466161486   T   T   T
  9.5993427345541118 10.2439325036104343  8.0000000000000000   F   F   F
  7.6795022269546820 12.8037186561727250  8.0000055199296689   F   F   F
  9.5993426244336906 12.1849137107467609  8.0000008619369254   F   F   F
  7.6795029569933133 14.7446998663250284  8.0000049280612373   F   F   F
  6.7195777971110386 10.2439325223392945  9.6370125635575086   F   F   F
 10.5592561205869622 12.8037186749015852  9.6370180834871775   F   F   F
  6.7195776869906165 12.1849137294756229  9.6370134254944340   F   F   F
 10.5592568506255962 14.7446998850538904  9.6370174916187459   F   F   F
  9.5667951910065216 10.2020791832588795 11.3345026063691723   T   T   T
  7.7136637833477417 12.7628531440949295 11.3351243913384359   T   T   T
  9.6138804574251129 12.1941200485831036 11.3132562736472035   T   T   T
  7.6668691436375616 14.7546555727145758 11.3129069773853157   T   T   T
  6.5026242435111294 10.3434202343553387 12.7302159439035929   T   T   T
 10.7760404832442074 12.9017581949622837 12.7279491417207158   T   T   T
  6.7680788219024981 12.2015568131580974 12.9667951780707931   T   T   T
 10.5120516416254670 14.7603299969040034 12.9652132921030638   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Ir E_tot= -603.65985652
eV
 D3-zero damping= -29.7683214 eV, D3-BJ damping= -32.2665942 eV
Ir
 1.0000000000000000
    11.5190376621507102    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.3587168828676166    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7019145515794847
  72
Cartesian
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  1.9198063027507983 -0.0000000000000000  7.9967732525545827
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Interface: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Rh E_tot= -938.56637604 eV
D3-zero damping= -49.7513981 eV, D3-BJ damping= -53.3107943 eV

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Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
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2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2  72
Selective dynamics
Cartesian
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  9.4636771258674450  3.7073751101412311 18.7025071161719332   T   T   T
  7.6406197786200023  9.4362910323590512 15.1766879143014091   T   T   T
  9.4042669348541121  7.5639854871132153 15.2098597619979312   T   T   T
  7.5543498992214060  7.5573654881582835 17.0388590042988319   T   T   T
  9.4825168112942642  9.4658519642779133 17.0176760902286297   T   T   T
  7.5264711980402828  9.4954865939377253 18.7731676113838652   T   T   T
  9.5120980841460305  7.5492788408850506 18.7893989450745487   T   T   T
  7.5828112692125789 13.1754663857249348 14.8539240643494672   T   T   T
  9.4272668176744006 11.3167992865256437 15.1032197751082666   T   T   T
  7.5522867934865268 11.3690831612496392 16.9328821736582427   T   T   T
  9.4324899755275613 13.2730180459841076 16.8004472762431156   T   T   T
  7.5787277033164866 13.3022429571312131 18.6805683394628197   T   T   T
  9.4690294193953051 11.4173210769001745 18.7302293286124595   T   T   T

Oxide reference: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Rh E_tot= -417.81573451
eV
 D3-zero damping= -12.9898376 eV, D3-BJ damping= -14.8349812 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn
O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O
 1.0000000000000000
    11.3603606973764180    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.1471475965018918    0.0000000000000000
     0.0000000000000000    0.0000000000000000   21.0215246346559006
```

```
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2
2   2   2   2   2   2   2   2   2   2   2
Selective dynamics
Cartesian
  3.7869292644155319  0.0047219605793061  8.0000000000000000   F   F   F
  1.8935349299714830  2.5292465653393479  8.0000055199296671   F   F   F
  3.7869291558120404  1.9189657773480042  8.0000008619369254   F   F   F
  1.8935356499536939  4.4434903850824794  8.0000049280612373   F   F   F
  0.9468336442313438  0.0047219790501744  9.6370125635575068   F   F   F
  4.7336196584755035  2.5292465838102163  9.6370180834871757   F   F   F
  0.9468335356278514  1.9189657958188724  9.6370134254944340   F   F   F
  4.7336203784577142  4.4434904035533469  9.6370174916187459   F   F   F
  3.7710680211681047 -0.0512434460654978 11.3543013910804831   T   T   T
  1.9116491685468877  2.4714480263830230 11.3531656965383867   T   T   T
  3.8157984487622807  1.9348900614011899 11.3293193287429297   T   T   T
  1.8655398584065073  4.4577738075995539 11.3285737258889885   T   T   T
  0.7574210585079149  0.0837535588388722 12.7917405065933067   T   T   T
  4.9299419513865583  2.6098403030448849 12.7940190645126837   T   T   T
  1.0183627487679219  1.9455879588313283 13.0259214094313922   T   T   T
  4.6629819921353768  4.4707610470535757 13.0276241709145033   T   T   T
  3.7869294266349582  5.0537711594132677  8.0000000000000000   F   F   F
  1.8935350921909098  7.5782957641733093  8.0000055199296671   F   F   F
  3.7869293180314672  6.9680149761819665  8.0000008619369254   F   F   F
  1.8935358121731207  9.4925395839164430  8.0000049280612373   F   F   F
  0.9468338064507703  5.0537711778841361  9.6370125635575068   F   F   F
  4.7336198206949307  7.5782957826441795  9.6370180834871757   F   F   F
  0.9468336978472782  6.9680149946528349  9.6370134254944340   F   F   F
  4.7336205406771414  9.4925396023873070  9.6370174916187459   F   F   F
  3.7700698567159949  4.9945855266907913 11.3541751397749024   T   T   T
  1.9093749470827499  7.5222122342521089 11.3542694975557232   T   T   T
  3.8123287839296442  6.9809941399001323 11.3268869122765015   T   T   T
  1.8646489710489997  9.5083881883970438 11.3292470287186120   T   T   T
  0.7524334601464931  5.1336853661144328 12.7922841035618493   T   T   T
  4.9229569332764420  7.6574678498810833 12.7917146323968485   T   T   T
  1.0134452427811727  6.9955994490137199 13.0252497530515789   T   T   T
  4.6621328115647875  9.5192607041662889 13.0260101114771238   T   T   T
  3.7869295888543850 10.1028203582472305  8.0000000000000000   F   F   F
  1.8935352544103363 12.6273449630072729  8.0000055199296671   F   F   F
  3.7869294802508939 12.0170641750159302  8.0000008619369254   F   F   F
  1.8935359743925473 14.5415887827504022  8.0000049280612373   F   F   F
  0.9468339686701970 10.1028203767180980  9.6370125635575068   F   F   F
  4.7336199829143570 12.6273449814781387  9.6370180834871757   F   F   F
  0.9468338600667049 12.0170641934867959  9.6370134254944340   F   F   F
  4.7336207028965678 14.5415888012212715  9.6370174916187459   F   F   F
  3.7687910133883844 10.0449109849883627 11.3531842003069681   T   T   T
  1.9103919969221337 12.5680921009829678 11.3541698508580833   T   T   T
  3.8148659863053438 12.0312291972095213 11.3284879063041259   T   T   T
  1.8681207489572154 14.5545138820829472 11.3268968380536172   T   T   T
  0.7506067146266756 10.1832580247572828 12.7940854934599386   T   T   T
  4.9278627546798610 12.7071341180616475 12.7922986953163953   T   T   T
  1.0173561295820110 12.0443234307664326 13.0275547153261240   T   T   T
  4.6670062644543613 14.5689806568372386 13.0252172149863465   T   T   T
  9.4671096131037409  0.0047219605793061  8.0000000000000000   F   F   F
  7.5737152786596926  2.5292465653393479  8.0000055199296671   F   F   F
  9.4671095045002502  1.9189657773480042  8.0000008619369254   F   F   F
  7.5737159986419007  4.4434903850824794  8.0000049280612373   F   F   F
  6.6270139929195508  0.0047219790501744  9.6370125635575068   F   F   F
 10.4138000071637133  2.5292465838102163  9.6370180834871757   F   F   F
  6.6270138843160602  1.9189657958188724  9.6370134254944340   F   F   F
 10.4138007271459223  4.4434904035533469  9.6370174916187459   F   F   F
  9.4512483698563372 -0.0512434705892420 11.3543013910804831   T   T   T
  7.5918295172350883  2.4714480263830230 11.3531656965383867   T   T   T
```

```
  9.4959787974505154  1.9348900614011899 11.3293193287429297   T   T   T
  7.5457202070947220  4.4577738075995539 11.3285737258889885   T   T   T
  6.4376013709763500  0.0837535876267299 12.7917404820695619   T   T   T
 10.6101223000748028  2.6098403030448849 12.7940190645126837   T   T   T
  6.6985430974561435  1.9455879833550729 13.0259214094313922   T   T   T
 10.3431623408236071  4.4707610470535757 13.0276241709145033   T   T   T
  9.4671097753231663  5.0537711594132677  8.0000000000000000   F   F   F
  7.5737154408791190  7.5782957641733093  8.0000055199296671   F   F   F
  9.4671096667196739  6.9680149761819665  8.0000008619369254   F   F   F
  7.5737161608613288  9.4925395839164430  8.0000049280612373   F   F   F
  6.6270141551389781  5.0537711778841361  9.6370125635575068   F   F   F
 10.4138001693831406  7.5782957826441795  9.6370180834871757   F   F   F
  6.6270140465354865  6.9680149946528349  9.6370134254944340   F   F   F
 10.4138008893653495  9.4925396023873070  9.6370174916187459   F   F   F
  9.4502502054041813  4.9945856048922979 11.3541751397749024   T   T   T
  7.5895552957709480  7.5222122852862361 11.3542694975557232   T   T   T
  9.4925091326178297  6.9809941998640008 11.3268869122765015   T   T   T
  7.5448292952134803  9.5083882234470760 11.3292470532423568   T   T   T
  6.4326138088347049  5.1336853661144328 12.7922841035618493   T   T   T
 10.6031373107525599  7.6574679526063347 12.7917146323968485   T   T   T
  6.6936256159930982  6.9955994735374638 13.0252497530515789   T   T   T
 10.3423131890408460  9.5192607329541499 13.0260101114771238   T   T   T
  9.4671099375425936 10.1028203582472305  8.0000000000000000   F   F   F
  7.5737156030985471 12.6273449630072729  8.0000055199296671   F   F   F
  9.4671098289391029 12.0170641750159302  8.0000008619369254   F   F   F
  7.5737163230807552 14.5415887827504022  8.0000049280612373   F   F   F
  6.6270143173584053 10.1028203767180980  9.6370125635575068   F   F   F
 10.4138003316025642 12.6273449814781387  9.6370180834871757   F   F   F
  6.6270142087549138 12.0170641934867959  9.6370134254944340   F   F   F
 10.4138010515847785 14.5415888012212715  9.6370174916187459   F   F   F
  9.4489713620766622 10.0449109238594190 11.3531842003069681   T   T   T
  7.5905723701340770 12.5680921009829678 11.3541698508580833   T   T   T
  9.4950463349935568 12.0312292040015194 11.3284879063041259   T   T   T
  7.5483010731216851 14.5545139066066920 11.3268968380536172   T   T   T
  6.4307870122807635 10.1832580247572828 12.7940854934599386   T   T   T
 10.6080431033680611 12.7071341962631497 12.7922987735178957   T   T   T
  6.6975364782702300 12.0443234307664326 13.0275547153261240   T   T   T
 10.3471866376662831 14.5689806244961506 13.0252172395100914   T   T   T

Metal reference: ZnO(11-20)/fcc(100)_3sqrt2x4sqrt2/Rh E_tot= -497.30117733
eV
 D3-zero damping= -24.0500513 eV, D3-BJ damping= -29.0035003 eV
Rh
 1.0000000000000000
    11.3603606973764180    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.1471475965018918    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.6769572608397070
  72
Cartesian
 -0.0000000255181879  1.8933934561212453  7.9956110468895547
  1.8924151127996092  0.0000000221428253  7.9966945789762187
  0.0000000348027771  0.0000000638273244  9.8384786869859511
  1.8927745440461023  1.8933934469563785  9.8384786304484457
  0.0000000726373658  1.8933934495627365 11.6813462506311492
  1.8924150906177810  0.0000000352690823 11.6802626382344421
 -0.0000000125049744  5.6801803419184145  7.9956111579980211
  1.8924150722976545  3.7867868800056823  7.9966946701288490
 -0.0000000082406749  3.7867868999990493  9.8384786795131660
  1.8927745254135127  5.6801803377198823  9.8384786586204900
  0.0000000788651140  5.6801803486882090 11.6813462013614195
  1.8924150629758294  3.7867868825891136 11.6802625270119176
 -0.0000000225339591  9.4669672607441573  7.9956110758379788
  1.8924150798747414  7.5735737982509459  7.9966947289152808
```

```
  0.0000000194683409  7.5735738125802730  9.8384786562817741
  1.8927745291333584  9.4669672610028908  9.8384787232788398
  0.0000000049555772  9.4669673065983666 11.6813462977461491
  1.8924150942727673  7.5735738197322116 11.6802626004965884
 -0.0000000089818281 13.2537541569170063  7.9956109946161673
  1.8924151224010608 11.3603606950042746  7.9966946748009216
  0.0000000252221310 11.3603606559767449  9.8384787122680084
  1.8927746386046620 13.2537541570810546  9.8384787273030376
  0.0000000049555772 13.2537541490741653 11.6813464022603970
  1.8924150930676604 11.3603606786436995 11.6802626918692187
  3.7877652445368533  1.8933934578584215  7.9966946364580727
  5.6801804522632882 -0.0000000187327226  7.9956110459004890
  3.7874058354361226  0.0000000363387935  9.8384786376719315
  5.6801803289027948  1.8933934213522741  9.8384785263946508
  3.7877652027438491  1.8933934702854582 11.6802626206093141
  5.6801803652245679 -0.0000000187327226 11.6813462099673995
  3.7877652881567152  5.6801803687266998  7.9966947023228183
  5.6801803706365552  3.7867868930091313  7.9956109918364220
  3.7874058131721253  3.7867868847684565  9.8384786073504724
  5.6801803316284145  5.6801803419062473  9.8384785862745474
  3.7877652218073328  5.6801803251726000 11.6802625963109659
  5.6801803205041734  3.7867868822127155 11.6813462332537181
  3.7877652486924358  9.4669672465079184  7.9966946967404295
  5.6801803486882090  7.5735737808930921  7.9956110262060021
  3.7874058473604535  7.5735738279529299  9.8384786541455753
  5.6801803001785354  9.4669672642034044  9.8384786407026272
  3.7877652121108065  9.4669672775906299 11.6802626243816334
  5.6801803030491618  7.5735738161544273 11.6813462629642757
  3.7877653287485775 13.2537541491355171  7.9966947494652283
  5.6801803486882090 11.3603606703586824  7.9956111322362222
  3.7874058029335509 11.3603606725550481  9.8384787324655942
  5.6801804018856927 13.2537541316175069  9.8384786108688509
  3.7877652287195667 13.2537541188887147 11.6802625468055759
  5.6801803979423937 11.3603606951800575 11.6813461831420895
  7.5725954491294871  1.8933934779491910  7.9966946686797664
  9.4679456345666146  0.0000000104477070  7.9966947296356201
  7.5729548957486355 -0.0000000486149732  9.8384785622012014
  9.4675861380296915  1.8933934385185058  9.8384786501942028
  7.5725954723347613  1.8933934564976442 11.6802625208185678
  9.4679456046236297 -0.0000000211434620 11.6802626345362945
  7.5725954092197076  5.6801803383483342  7.9966946191218726
  9.4679456450091823  3.7867869298840748  7.9966947233637953
  7.5729548886120766  3.7867869076184402  9.8384785549636700
  9.4675861909190928  5.6801803713789907  9.8384786543581786
  7.5725953944969371  5.6801803285127104 11.6802626110494359
  9.4679456672923852  3.7867869275119279 11.6802626022835412
  7.5725954601737149  9.4669672125446027  7.9966947153771546
  9.4679456548280321  7.5735737781495063  7.9966947182786106
  7.5729548161462583  7.5735737758684154  9.8384785926812288
  9.4675861814836626  9.4669672437593686  9.8384786225669814
  7.5725954019659509  9.4669672839733572 11.6802625715152679
  9.4679456009686422  7.5735738037430780 11.6802626277241206
  7.5725954710421659 13.2537541161805503  7.9966947695945416
  9.4679455749753547 11.3603606950042746  7.9966947330362688
  7.5729548319383326 11.3603607326874396  9.8384785059807420
  9.4675861121670195 13.2537541931535099  9.8384785974366302
  7.5725954085244593 13.2537540893722667 11.6802624935065680
  9.4679455835928330 11.3603607084206484 11.6802626883042073

Interface: TiO2(110)/fcc(100)_sqrt5/Au E_tot= -473.10241728 eV
 D3-zero damping= -15.3918239 eV, D3-BJ damping= -17.3217989 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Au
 1.0000000000000000
```

```
     6.4818058745047109    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.4818058745047109    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.2947969373044117
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000007  1.6204514686261784  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.9720246192593140  1.6204514686261784  9.2861208469999994   F   F   F
  3.2409029372523563  0.0000000000000006  9.2861208469999994   F   F   F
  3.2409029372523563  1.6204514686261788 12.5708101129999967   F   F   F
  3.2409029372523563  0.0000000000000008 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000024   F   F   F
  4.5097812552453984  1.6204514686261784  9.2861208469999994   F   F   F
  5.2129275565116693  1.6204514686261788 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000008 12.5708101129999967   F   F   F
  6.4861218514411707  1.4577077360214927 15.7083909483763868   T   T   T
 -0.0050882805975555 -0.0337405384514121 14.5752193745609819   T   T   T
  3.2409029372523563  0.0000000000000009 13.8569309599999961   F   F   F
  1.2688783179930430  1.6204514686261788 12.5708101129999967   F   F   F
  1.9315879843827399  1.6243806770893505 15.7901174672965148   T   T   T
  3.2433013923142191 -0.2512301882631324 15.7927435086095649   T   T   T
  3.3030120706088351  1.3287460211329041 19.0974578710829412   T   T   T
  3.2760522396146019  0.0556913715540909 17.6856629939320591   T   T   T
  6.4778810429381846  0.0330266417258701 17.1050952697120628   T   T   T
  4.5564874536121351  1.6417619313130538 15.7926415418724044   T   T   T
  5.2796173379381406  1.6228197495605641 19.1352980287316363   T   T   T
  0.1292184258954347  0.0714302204321833 18.9205282035360405   T   T   T
  3.2903865536560861 -0.1323999890134572 20.2035332740471922   T   T   T
  1.2826828082907684  1.5106714813415554 19.1165514864721864   T   T   T
  0.0000000000000008  4.8613544058785330  9.2861208469999994   F   F   F
  0.0000000000000007  3.2409029372523563  8.0000000000000000   F   F   F
  1.9720246192593143  4.8613544058785330  9.2861208469999994   F   F   F
  3.2409029372523563  3.2409029372523563  9.2861208469999994   F   F   F
  3.2409029372523563  4.8613544058785330 12.5708101129999967   F   F   F
  3.2409029372523563  3.2409029372523563 11.2846892659999973   F   F   F
  0.0000000000000008  3.2409029372523563 10.5722416940000024   F   F   F
  4.5097812552453984  4.8613544058785330  9.2861208469999994   F   F   F
  5.2129275565116693  4.8613544058785330 12.5708101129999967   F   F   F
  0.0000000000000009  3.2409029372523563 12.5708101129999967   F   F   F
  6.4782458401165890  4.7006230208872779 15.7072791215710410   T   T   T
  0.0053364923236534  3.2009541316954868 14.5782688724369489   T   T   T
  3.2409029372523563  3.2409029372523563 13.8569309599999961   F   F   F
  1.2688783179930432  4.8613544058785330 12.5708101129999967   F   F   F
  1.9243900855666276  4.8880984302913788 15.7810035326434921   T   T   T
  3.2399976139062652  2.9891212466011385 15.7876954069285294   T   T   T
  3.1912068762645829  4.5832830188115885 19.0866663315547243   T   T   T
  3.2139716520897901  3.3389558884588069 17.6656405509120802   T   T   T
  6.4877927719248456  3.2871674989615416 17.1120443734065830   T   T   T
  4.5529457405075693  4.8693976130435299 15.7757824850128685   T   T   T
  5.2079120198396760  4.7534732670096789 19.1461464930382732   T   T   T
 -0.1155547228975620  3.3141624504010614 18.9261488561930697   T   T   T
  3.1964186822520464  3.0920607362729551 20.1627847485516831   T   T   T
  1.2077334213775957  4.8634754525414081 19.1559473086379164   T   T   T
  0.5790984176826807  6.0858611846182491 24.2730001158119180   T   T   T
 -0.0634216566143001  1.5626112014929339 21.9960834819900981   T   T   T
  1.9499502274230005  2.1642525143074867 24.1434082053209202   T   T   T
 -0.0477961719792104  1.5147677692202555 26.3010189835496462   T   T   T
  1.1569179040328863  4.0056549096817635 22.1342234592020297   T   T   T
  3.1940262020790589  4.7785889943621811 24.2198682987627656   T   T   T
  1.2602792117411883  4.0864609662892564 26.2687846110956968   T   T   T
  2.3020236352375782  6.5726994484370413 22.1842952012618646   T   T   T
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  4.4511978344080978  7.3328678207568636 24.0748942899487339   T   T   T
  2.5749626001925323  6.7109709419086672 26.2928254669759447   T   T   T
  4.0416662704317003  3.0211142150554928 22.1987752755828538   T   T   T
  5.7917058716052612  3.4320454972268175 24.2734780252605979   T   T   T
  3.8283810991458895  2.8027899488218027 26.2977709910004656   T   T   T
  5.3388006909845069  5.5237059897388612 22.0309823868456185   T   T   T
  5.1283174229663757  5.4299484192939449 26.2718332066597959   T   T   T

Oxide reference: TiO2(110)/fcc(100)_sqrt5/Au E_tot= -420.23636211 eV
 D3-zero damping= -6.3299627 eV, D3-BJ damping= -9.0768408 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
     6.4818058745047109    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.4818058745047109    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.4848354988443120
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000007  1.6204514686261784  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.9720246192593140  1.6204514686261784  9.2861208469999994   F   F   F
  3.2409029372523563  0.0000000000000006  9.2861208469999994   F   F   F
  3.2409029372523563  1.6204514686261788 12.5708101129999967   F   F   F
  3.2409029372523563  0.0000000000000008 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000006   F   F   F
  4.5097812552453984  1.6204514686261784  9.2861208469999994   F   F   F
  5.2129275565116693  1.6204514686261788 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000008 12.5708101129999967   F   F   F
  6.4852073305220470  1.4759103996272742 15.6937858004621749   T   T   T
 -0.0030733602515667 -0.0332456346829425 14.5409694657315516   T   T   T
  3.2409029372523563  0.0000000000000009 13.8569309599999961   F   F   F
  1.2688783179930430  1.6204514686261788 12.5708101129999967   F   F   F
  1.9237059347237040  1.6325120967179578 15.7749518281273815   T   T   T
  3.2488426451131978 -0.2265204046812755 15.8557872705965845   T   T   T
  3.3008829384699010  1.1641265664222453 19.2747685328000067   T   T   T
  3.2790632396238424  0.0932244719687928 17.6730261240443411   T   T   T
  6.4941167087738174 -0.0178848243927869 17.0513666995651398   T   T   T
  4.5626887452951390  1.6413568375109260 15.7775389720200678   T   T   T
  5.3098754224839517  1.4685617751998881 19.1761187163809517   T   T   T
  0.1117671510581236 -0.0193216688722567 18.8646386298459845   T   T   T
  3.2774590758849986 -0.3264597319867638 20.2576048166244860   T   T   T
  1.2783889635921388  1.3757329979945758 19.1480155917216592   T   T   T
  0.0000000000000008  4.8613544058785330  9.2861208469999994   F   F   F
  0.0000000000000007  3.2409029372523563  8.0000000000000000   F   F   F
  1.9720246192593143  4.8613544058785330  9.2861208469999994   F   F   F
  3.2409029372523563  3.2409029372523563  9.2861208469999994   F   F   F
  3.2409029372523563  4.8613544058785330 12.5708101129999967   F   F   F
  3.2409029372523563  3.2409029372523563 11.2846892659999973   F   F   F
  0.0000000000000008  3.2409029372523563 10.5722416940000006   F   F   F
  4.5097812552453984  4.8613544058785330  9.2861208469999994   F   F   F
  5.2129275565116693  4.8613544058785330 12.5708101129999967   F   F   F
  0.0000000000000009  3.2409029372523563 12.5708101129999967   F   F   F
  6.4838422739450809  4.7166860915884685 15.6938455566213459   T   T   T
  0.0074866350887478  3.2076789346383729 14.5409468374077750   T   T   T
  3.2409029372523563  3.2409029372523563 13.8569309599999961   F   F   F
  1.2688783179930432  4.8613544058785330 12.5708101129999967   F   F   F
  1.9233005816418600  4.8825493131421149 15.7784449232325059   T   T   T
  3.2383197478735326  3.0146067104594478 15.8554618803303846   T   T   T
  3.1867044828350299  4.4049757462517167 19.2747848120982823   T   T   T
  3.2099826399721718  3.3345133413800143 17.6730377231900881   T   T   T
  6.4740600291689887  3.2231388224294957 17.0509704518067018   T   T   T
  4.5626785767628206  4.8730697623253301 15.7745646773879642   T   T   T
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  5.2105521838558051  4.6176267934943249 19.1489656343041474   T   T   T
 -0.1063106807872796  3.2218928808407301 18.8645121473515083   T   T   T
  3.2119672906689898  2.9144084539130235 20.2577590728670778   T   T   T
  1.1791421065854046  4.7088960546225680 19.1761123029142659   T   T   T

Metal reference: TiO2(110)/fcc(100)_sqrt5/Au E_tot= -49.9060994 eV
 D3-zero damping= -6.1516271 eV, D3-BJ damping= -6.205904 eV
Au
 1.0000000000000000
     6.4818058745047109    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.4818058745047109    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9667868910931077
  15
Cartesian
  0.6486111856774751  4.5358827144140994 10.0148680382787116
 -0.0000037520671300 -0.0000128328400971  7.9350973572967733
  1.9445184794908259  0.6476442234373847 10.0135537917027175
 -0.0000217164930951  0.0000171717012321 12.0965914885755979
  1.2940834042336227  2.5935624345234358  7.9295751685569140
  3.2408786222516195  3.2409059811592487 10.0126226603353174
  1.2995024795040235  2.5905600234457435 12.0965319519769263
  2.5975681060283144  5.1850481063616929  7.9276122970221623
  4.5372850566091634  5.8341329014948329 10.0135545248631210
  2.5891207283529614  5.1872231218413622 12.0976259554914698
  3.8842702397278361  1.2967518408091638  7.9276321413203767
  5.8332051371312925  1.9459568416629129 10.0148552722388384
  3.8927325224441307  1.2946486179901626 12.0976103242783619
  5.1877235891475264  3.8882208310768283  7.9295775942981335
  5.1823743745745023  3.8912389432056020 12.0965700013616484

Interface: TiO2(110)/fcc(100)_sqrt5/Ag E_tot= -465.15976458 eV
 D3-zero damping= -13.6485267 eV, D3-BJ damping= -16.7987567 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ag
 1.0000000000000000
     6.4410542991872699    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.4410542991872699    0.0000000000000000
     0.0000000000000000    0.0000000000000000   33.7197606010724655
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000006  1.6102635747968181  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.9596263599847359  1.6102635747968181  9.2861208469999994   F   F   F
  3.2205271495936358  0.0000000000000006  9.2861208469999994   F   F   F
  3.2205271495936358  1.6102635747968186 12.5708101129999967   F   F   F
  3.2205271495936358  0.0000000000000008 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000024   F   F   F
  4.4814279392025353  1.6102635747968181  9.2861208469999994   F   F   F
  5.1801535095783704  1.6102635747968186 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000008 12.5708101129999967   F   F   F
  6.4435624762187276  1.7068610500859980 15.6941571704992171   T   T   T
  0.0058118623063688  0.0108954414210560 14.5901925781646540   T   T   T
  3.2205271495936358  0.0000000000000009 13.8569309599999961   F   F   F
  1.2609007896089006  1.6102635747968186 12.5708101129999967   F   F   F
  1.9292860356036541  1.5967663984988048 15.7842436409585911   T   T   T
  3.2326048037539827 -0.2443745808828314 15.7855829654332442   T   T   T
  3.2284716138775780  1.2897778814183687 19.0865106860745257   T   T   T
  3.2253868506150223  0.0638865704900685 17.6648024544723441   T   T   T
  6.4406641218177860 -0.1079901139624138 17.1356677423571284   T   T   T
  4.5150587998837395  1.5910369448060764 15.7768060715435112   T   T   T
  5.2147821453323076  1.5093874664016946 19.2305753023482104   T   T   T
  0.0753118010766962 -0.1799192634391532 18.9343453220060098   T   T   T
```

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  3.2504374667590756 -0.2069365363595533 20.1476480785109970   T   T   T
  1.2132024681199001  1.4435934914234727 19.2666091731885025   T   T   T
  0.0000000000000008  4.8307907243904520  9.2861208469999994   F   F   F
  0.0000000000000007  3.2205271495936358  8.0000000000000000   F   F   F
  1.9596263599847361  4.8307907243904520  9.2861208469999994   F   F   F
  3.2205271495936358  3.2205271495936358  9.2861208469999994   F   F   F
  3.2205271495936358  4.8307907243904520 12.5708101129999967   F   F   F
  3.2205271495936358  3.2205271495936358 11.2846892659999973   F   F   F
  0.0000000000000008  3.2205271495936358 10.5722416940000024   F   F   F
  4.4814279392025353  4.8307907243904520  9.2861208469999994   F   F   F
  5.1801535095783704  4.8307907243904520 12.5708101129999967   F   F   F
  0.0000000000000009  3.2205271495936358 12.5708101129999967   F   F   F
  6.4507638256496103  4.9223684414828348 15.6923955534272821   T   T   T
  0.0033430882298486  3.2432863134981225 14.5886454510341288   T   T   T
  3.2205271495936358  3.2205271495936358 13.8569309599999961   F   F   F
  1.2609007896089008  4.8307907243904520 12.5708101129999967   F   F   F
  1.9367021678792944  4.7946194719482227 15.8107296238148116   T   T   T
  3.2232561800879842  2.9853833978255655 15.7981375263622663   T   T   T
  3.2360609192837466  4.4666731373596429 19.1526495584213023   T   T   T
  3.2380722555836794  3.1979430320582836 17.7365893711652731   T   T   T
  6.4412246604080190  3.0961081039800082 17.1438691051434731   T   T   T
  4.5156737396800226  4.7938058523625564 15.8047267446915338   T   T   T
  5.2419331051992604  4.6638102218890065 19.2755055606724461   T   T   T
 -0.0452546120921787  3.0422058555015106 18.9462539152956033   T   T   T
  3.1899579403105967  3.0330177924797104 20.2982668138555660   T   T   T
  1.2383785826339284  4.7087260161439053 19.1908560626153673   T   T   T
  1.1798025579073514  5.5942015472671249 24.1613225423286622   T   T   T
  0.5566925593304614  1.0756744369381301 22.0349359251091421   T   T   T
  2.4958113336090495  1.7572795140699256 24.1768279801790875   T   T   T
  0.5638479017553255  1.0883748687994006 26.2177528718255459   T   T   T
  1.7479607541577220  3.6354041002921824 22.0935977781312971   T   T   T
  3.7777939627630990  4.2921619704161067 24.1715133700678670   T   T   T
  1.8453800338340736  3.6671970818152784 26.2324081012800256   T   T   T
  3.1176176879732780  6.2447546573060420 22.2847333129509231   T   T   T
  5.0840499011973366  6.8939027482271893 24.1583684805116512   T   T   T
  3.1358815477189026  6.2408909108312924 26.2302764240642183   T   T   T
  4.5279180229375129  2.4138759273669259 22.1059298785809624   T   T   T
  6.3585322185894126  3.0260016093338638 24.1457523624123027   T   T   T
  4.4268712251908093  2.3753648602827262 26.2326779792431104   T   T   T
  5.7212564990450305  4.9931390319723157 22.0180975710426274   T   T   T
  5.7045952222272538  4.9540736126211353 26.2181858100622875   T   T   T

Oxide reference: TiO2(110)/fcc(100)_sqrt5/Ag E_tot= -420.71525269 eV
 D3-zero damping= -6.3900941 eV, D3-BJ damping= -9.2002908 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
     6.4410542991872699    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.4410542991872699    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.4848354988443120
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.6102635747968181  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.9596263599847359  1.6102635747968181  9.2861208469999994   F   F   F
  3.2205271495936358  0.0000000000000006  9.2861208469999994   F   F   F
  3.2205271495936358  1.6102635747968186 12.5708101129999967   F   F   F
  3.2205271495936358  0.0000000000000008 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000006   F   F   F
  4.4814279392025353  1.6102635747968181  9.2861208469999994   F   F   F
  5.1801535095783704  1.6102635747968186 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000008 12.5708101129999967   F   F   F
```

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  6.4407754816631169  1.6102635622554298 15.6726626501332191   T   T   T
  0.0001182715110362  0.0000000000000010 14.5554691333024131   T   T   T
  3.2205271495936358  0.0000000000000009 13.8569309599999961   F   F   F
  1.2609007896089006  1.6102635747968186 12.5708101129999967   F   F   F
  1.9330322403832307  1.6102635747968186 15.8089153068384078   T   T   T
  3.2198227111464206  0.0000000845106044 15.9131867601843862   T   T   T
  3.2205692054256652  1.6102647120743725 19.2615303925006529   T   T   T
  3.2205834363272547 -0.0000006822331698 17.7443795730214831   T   T   T
  6.4411616147673749  0.0000000000000011 17.0480001212098600   T   T   T
  4.5085477422087346  1.6102633528652819 15.8088072492062892   T   T   T
  5.2350042350757464  1.6102642097197646 19.1336369222964287   T   T   T
  0.0000306662694833  0.0000000000000013 18.8418511724888802   T   T   T
  3.2205392085114974  0.0000002231979868 20.2413204631926398   T   T   T
  1.2060974480519575  1.6102630029997820 19.1336403513042228   T   T   T
  0.0000000000000008  4.8307907243904520  9.2861208469999994   F   F   F
  0.0000000000000007  3.2205271495936358  8.0000000000000000   F   F   F
  1.9596263599847361  4.8307907243904520  9.2861208469999994   F   F   F
  3.2205271495936358  3.2205271495936358  9.2861208469999994   F   F   F
  3.2205271495936358  4.8307907243904520 12.5708101129999967   F   F   F
  3.2205271495936358  3.2205271495936358 11.2846892659999973   F   F   F
  0.0000000000000008  3.2205271495936358 10.5722416940000006   F   F   F
  4.4814279392025353  4.8307907243904520  9.2861208469999994   F   F   F
  5.1801535095783704  4.8307907243904520 12.5708101129999967   F   F   F
  0.0000000000000009  3.2205271495936358 12.5708101129999967   F   F   F
  6.4407754641176789  4.8307907369318448 15.6726626501332191   T   T   T
  0.0001182843637025  3.2205271495936358 14.5554691515886656   T   T   T
  3.2205271495936358  3.2205271495936358 13.8569309599999961   F   F   F
  1.2609007896089008  4.8307907243904520 12.5708101129999967   F   F   F
  1.9330322448713184  4.8307905676076635 15.8089153023745475   T   T   T
  3.2198219435833595  3.2205272341042388 15.9131867502194577   T   T   T
  3.2205692054256652  4.8307918959769758 19.2615303880368067   T   T   T
  3.2205834149481096  3.2205265116573600 17.7443795464986955   T   T   T
  6.4411613016572842  3.2205271495936358 17.0480001811380610   T   T   T
  4.5085477422087346  4.8307907243904520 15.8088072732645752   T   T   T
  5.2350042105841510  4.8307901496555390 19.1336369213936166   T   T   T
  0.0000251001688792  3.2205271495936363 18.8418512105983638   T   T   T
  3.2205388052689612  3.2205273797303473 20.2413204355998921   T   T   T
  1.2060974126998640  4.8307913853837459 19.1336404035142706   T   T   T

Metal reference: TiO2(110)/fcc(100)_sqrt5/Ag E_tot= -40.93432735 eV
 D3-zero damping= -4.4899851 eV, D3-BJ damping= -5.6514842 eV
Ag
 1.0000000000000000
     6.4410542991872699    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.4410542991872699    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9667868910931077
  15
Cartesian
  0.6453479702581829  4.5087729759674255 10.0137998760010642
 -0.0000045033806866  0.0000145159791113  7.9472067980345154
  1.9311607800442934  0.6439436611310140 10.0133628660769940
  0.0000110317189528  0.0000111248643734 12.0823089063102316
  1.2870430930650574  2.5763197852299928  7.9476587617307954
  3.2205287592998668  3.2205321480143287 10.0135868189314436
  1.2878982671634709  2.5774546450443636 12.0807360777401200
  2.5770677312494819  5.1533014593065634  7.9454510449936899
  4.5099107324367589  5.7971333675631671 10.0133727498494594
  2.5756892733334964  5.1541344580594890 12.0793557626770163
  3.8640059985663227  1.2877611048108257  7.9454426112700922
  5.7957167042676447  1.9322968059294672 10.0138145906055520
  3.8653709990747878  1.2869212390886280 12.0793647064289100
  5.1540486917665564  3.8646933040945819  7.9476736617475341
  5.1531663509902552  3.8636048121677731 12.0807438220264434
```

```
Interface: TiO2(110)/fcc(100)_sqrt5/Pt E_tot= -515.73130241 eV
 D3-zero damping= -16.9795888 eV, D3-BJ damping= -19.8261655 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Pt
 1.0000000000000000
     6.1949220535721867    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1949220535721867    0.0000000000000000
     0.0000000000000000    0.0000000000000000   33.7197606010724655
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000006  1.5487305133930473  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.8847430855788028  1.5487305133930473  9.2861208469999994   F   F   F
  3.0974610267860943  0.0000000000000006  9.2861208469999994   F   F   F
  3.0974610267860943  1.5487305133930478 12.5708101129999967   F   F   F
  3.0974610267860943  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000024   F   F   F
  4.3101789679933846  1.5487305133930473  9.2861208469999994   F   F   F
  4.9822041123648955  1.5487305133930478 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000008 12.5708101129999967   F   F   F
  6.1861083777340191  1.4503190625851219 15.9777517990520490   T   T   T
  0.0045180878800061 -0.0458699755859882 14.5704490618600264   T   T   T
  3.0974610267860943  0.0000000000000009 13.8569309599999961   F   F   F
  1.2127179412072919  1.5487305133930478 12.5708101129999967   F   F   F
  1.8761011453719534  1.6407040590472157 15.7161106552198042   T   T   T
  2.9221320383280056  0.0265648206598668 15.8033843714526405   T   T   T
  3.1227065328125638  1.4897986969823509 19.2627927668570891   T   T   T
  2.8570101071353231  0.1070135560601820 17.8062287068418641   T   T   T
  6.3992183668122289  0.0411922253051558 17.1331625217685151   T   T   T
  4.2814364453721483  1.4604162599178052 15.8355319185268151   T   T   T
  5.0204265966208173  1.3295731007343454 19.0038265544113969   T   T   T
  0.1903082555234556 -0.0617514920680165 19.2231454738982919   T   T   T
  2.9515172628425366 -0.2103654211042470 20.2699430624113468   T   T   T
  1.1564669272062309  1.7570725736410919 19.5939517052134740   T   T   T
  0.0000000000000008  4.6461915401791396  9.2861208469999994   F   F   F
  0.0000000000000006  3.0974610267860943  8.0000000000000000   F   F   F
  1.8847430855788030  4.6461915401791396  9.2861208469999994   F   F   F
  3.0974610267860943  3.0974610267860943  9.2861208469999994   F   F   F
  3.0974610267860943  4.6461915401791396 12.5708101129999967   F   F   F
  3.0974610267860943  3.0974610267860943 11.2846892659999973   F   F   F
  0.0000000000000008  3.0974610267860943 10.5722416940000024   F   F   F
  4.3101789679933846  4.6461915401791396  9.2861208469999994   F   F   F
  4.9822041123648955  4.6461915401791396 12.5708101129999967   F   F   F
  0.0000000000000009  3.0974610267860943 12.5708101129999967   F   F   F
  6.1760871268313924  4.6076973388153659 15.7262424127549512   T   T   T
 -0.0836674566506173  3.1421449242218475 14.5600335209175604   T   T   T
  3.0974610267860943  3.0974610267860943 13.8569309599999961   F   F   F
  1.2127179412072921  4.6461915401791396 12.5708101129999967   F   F   F
  1.8892326089913074  4.5679329436240028 15.8635078200386470   T   T   T
  3.2169171749115191  3.0854587088029692 15.8140919769899462   T   T   T
  3.0465832938279003  4.6389720735112565 18.7611892445652764   T   T   T
  3.0502984356301241  2.9801136743993157 17.7775375514910614   T   T   T
  6.1104627120828159  3.0260716593256962 17.1660544309343308   T   T   T
  4.2776851197628956  4.7272378935754720 15.9745657379128065   T   T   T
  4.9908489348166958  4.8942206116737328 18.8092927823289067   T   T   T
 -0.3904262834062513  3.1261671283538823 19.0361146257929974   T   T   T
  3.8362718292407987  3.2158755048535101 20.0242040679972391   T   T   T
  1.1574577508468822  4.4240332931314406 19.1694593237999698   T   T   T
  0.3668837364642842  3.8948560114873212 23.7871921616229436   T   T   T
 -0.1906764994294914 -0.3291209757617464 21.7173066092234315   T   T   T
  1.6206478378686591  0.2492632688914273 23.8262710267326625   T   T   T
```

```
 -0.2265680841376454 -0.4374374781979774 25.7634890375149972   T   T   T
  1.0131634206387972  2.1477404262464876 21.7113900524394268   T   T   T
  2.8814937736326613  2.6985910035838958 23.8020925200047593   T   T   T
  1.0108298824731308  2.0428701614465918 25.7869412745590481   T   T   T
  2.1574551983814758  4.5885567382555763 21.9483052852260627   T   T   T
  4.1185338507220521  5.1809111915698356 23.8350089356176937   T   T   T
  2.2278936925797055  4.5186833836443165 25.7452769980410707   T   T   T
  3.6180520556064470  0.9155053924332380 21.8891961022764967   T   T   T
  5.3770431090285360  1.4495196145830824 23.8238097031217180   T   T   T
  3.4985546608957936  0.8370501424038351 25.7454984474479147   T   T   T
  4.8235501522140920  3.4244123665471307 21.8160796027242405   T   T   T
  4.7420659650274279  3.3053316843801261 25.7685213440390690   T   T   T

Oxide reference: TiO2(110)/fcc(100)_sqrt5/Pt E_tot= -422.53916338 eV
 D3-zero damping= -6.7925965 eV, D3-BJ damping= -9.8682339 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
     6.1949220535721867    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1949220535721867    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.4848354988443120
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.5487305133930473  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.8847430855788028  1.5487305133930473  9.2861208469999994   F   F   F
  3.0974610267860943  0.0000000000000006  9.2861208469999994   F   F   F
  3.0974610267860943  1.5487305133930478 12.5708101129999967   F   F   F
  3.0974610267860943  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000006   F   F   F
  4.3101789679933846  1.5487305133930473  9.2861208469999994   F   F   F
  4.9822041123648955  1.5487305133930478 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000008 12.5708101129999967   F   F   F
  6.1949273543048706  1.5487305133930478 15.7022139308169919   T   T   T
  0.0000044174883102  0.0000000000000009 14.5630537247462435   T   T   T
  3.0974610267860943  0.0000000000000009 13.8569309599999961   F   F   F
  1.2127179412072919  1.5487305133930478 12.5708101129999967   F   F   F
  1.8747207078714045  1.5487305133930478 15.8783679234597255   T   T   T
  3.0974639232113237  0.0000000000000010 16.0140406798868327   T   T   T
  3.0974659467458885  1.5487305230876343 19.4130021370133932   T   T   T
  3.0974445570927394  0.0000000000000011 17.8602857168912657   T   T   T
  6.1949287199929097  0.0000000000000011 17.0950415058855363   T   T   T
  4.3202141289469074  1.5487305133930478 15.8783658655981430   T   T   T
  5.0317341939574245  1.5487305474836444 19.2368531308313813   T   T   T
  0.0000102034096280  0.0000000000000012 18.8902660788829486   T   T   T
  3.0974852629137599  0.0000000000000013 20.4507637230362604   T   T   T
  1.1631867851183904  1.5487304616025468 19.2369385045179015   T   T   T
  0.0000000000000008  4.6461915401791396  9.2861208469999994   F   F   F
  0.0000000000000006  3.0974610267860943  8.0000000000000000   F   F   F
  1.8847430855788030  4.6461915401791396  9.2861208469999994   F   F   F
  3.0974610267860943  3.0974610267860943  9.2861208469999994   F   F   F
  3.0974610267860943  4.6461915401791396 12.5708101129999967   F   F   F
  3.0974610267860943  3.0974610267860943 11.2846892659999973   F   F   F
  0.0000000000000008  3.0974610267860943 10.5722416940000006   F   F   F
  4.3101789679933846  4.6461915401791396  9.2861208469999994   F   F   F
  4.9822041123648955  4.6461915401791396 12.5708101129999967   F   F   F
  0.0000000000000009  3.0974610267860943 12.5708101129999967   F   F   F
  6.1949273583328708  4.6461915401791396 15.7022139826074874   T   T   T
  0.0000043980265336  3.0974610267860943 14.5630537423226443   T   T   T
  3.0974610267860943  3.0974610267860943 13.8569309599999961   F   F   F
  1.2127179412072921  4.6461915401791396 12.5708101129999967   F   F   F
  1.8747207185432953  4.6461915401791396 15.8783679234597255   T   T   T
```

```
  3.0974639060980733  3.0974610267860943 16.0140406782828819   T   T   T
  3.0974659280533099  4.6461915304845380 19.4130021086383096   T   T   T
  3.0974445035403657  3.0974610267860943 17.8602857449565917   T   T   T
  6.1949288397450584  3.0974610267860943 17.0950414893662526   T   T   T
  4.3202141364234405  4.6461915401791396 15.8783658655981430   T   T   T
  5.0317341551983414  4.6461915060885435 19.2368531935090523   T   T   T
  0.0000104372244201  3.0974610267860947 18.8902660619254057   T   T   T
  3.0974852357957618  3.0974610267860947 20.4507637847095509   T   T   T
  1.1631867380655447  4.6461915919696395 19.2369385353509941   T   T   T

Metal reference: TiO2(110)/fcc(100)_sqrt5/Pt E_tot= -89.57550119 eV
 D3-zero damping= -6.8911835 eV, D3-BJ damping= -7.2201746 eV
Pt
 1.0000000000000000
     6.1949220535721867    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1949220535721867    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9667868910931077
  15
Cartesian
  0.6197574200503924  4.3365269476953472 10.0138005312070852
 -0.0000795565715734  0.0000018997589199  8.0769264423456519
  1.8582455894286740  0.6199972109226815 10.0122180155136018
  0.0000529568400842  0.0000068401831580 11.9502625624664311
  1.2388259710458553  2.4786761512928255  8.0773707105591583
  3.0974828263097449  3.0974641742249651 10.0132231052315177
  1.2392382037991341  2.4773178217221767 11.9509654527743585
  2.4777843566869477  4.9557761292302569  8.0773457119706205
  4.3366780288174827  5.5749256126854272 10.0122548749389413
  2.4785197690043641  4.9564981040835940 11.9499920690953214
  3.7171028700646795  1.2391630908287616  8.0773501172137987
  5.5751887745660635  1.8584089567662725 10.0138160073834435
  3.7164366762706904  1.2384213706067182 11.9499744837667539
  4.9560988262932346  3.7162373917060632  8.0773821764420983
  4.9557655401616056  3.7176127123341014 11.9509965812100116

Interface: TiO2(110)/fcc(100)_sqrt5/Pd E_tot= -502.17842343 eV
 D3-zero damping= -15.1586033 eV, D3-BJ damping= -18.712701 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Pd
 1.0000000000000000
     6.1446728354220141    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1446728354220141    0.0000000000000000
     0.0000000000000000    0.0000000000000000   33.8893644244545840
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000006  1.5361682088555042  9.2861208469999976   F   F   F
  0.0000000000000005  0.0000000000000005  7.9999999999999982   F   F   F
  1.8694552634487942  1.5361682088555042  9.2861208469999976   F   F   F
  3.0723364177110080  0.0000000000000006  9.2861208469999976   F   F   F
  3.0723364177110080  1.5361682088555046 12.5708101129999950   F   F   F
  3.0723364177110080  0.0000000000000007 11.2846892659999956   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000006   F   F   F
  4.2752175719732213  1.5361682088555042  9.2861208469999976   F   F   F
  4.9417916811598008  1.5361682088555046 12.5708101129999950   F   F   F
  0.0000000000000007  0.0000000000000008 12.5708101129999950   F   F   F
  6.1201377645154089  1.7040600277722351 15.9424805190434284   T   T   T
 -0.0101457815793161  0.0125631762378185 14.5460811240015406   T   T   T
  3.0723364177110080  0.0000000000000009 13.8569309599999944   F   F   F
  1.2028811542622142  1.5361682088555046 12.5708101129999950   F   F   F
  1.8562189743375568  1.6052824574242437 15.7312770516512934   T   T   T
  2.9014853839072914 -0.0039810697294774 15.7958684395557682   T   T   T
  3.1383607234017759  1.4619085871034905 19.2953156410294149   T   T   T
```

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  2.7280918652166579  0.0470689532928327 17.8638267173450060   T   T   T
  6.3266236755295120  0.0422303920152255 17.0717986650087070   T   T   T
  4.2445724586859939  1.4187296757266097 15.9114517653367784   T   T   T
  5.0326005014241106  1.2754245454696354 19.0381509160905793   T   T   T
  0.3546129534560483 -0.0227084633123361 18.9319313204987765   T   T   T
  3.0547205525706387 -0.1710294802321775 20.3296376608982818   T   T   T
  1.1806685494171578  1.6869953794979409 19.6155355126827082   T   T   T
  0.0000000000000008  4.6085046265665106  9.2861208469999976   F   F   F
  0.0000000000000006  3.0723364177110080  7.9999999999999982   F   F   F
  1.8694552634487944  4.6085046265665106  9.2861208469999976   F   F   F
  3.0723364177110080  3.0723364177110080  9.2861208469999976   F   F   F
  3.0723364177110080  4.6085046265665106 12.5708101129999950   F   F   F
  3.0723364177110080  3.0723364177110080 11.2846892659999956   F   F   F
  0.0000000000000008  3.0723364177110080 10.5722416940000006   F   F   F
  4.2752175719732213  4.6085046265665106  9.2861208469999976   F   F   F
  4.9417916811598008  4.6085046265665106 12.5708101129999950   F   F   F
  0.0000000000000009  3.0723364177110080 12.5708101129999950   F   F   F
  6.1093900251919173  4.7338812675483508 15.7176474987312211   T   T   T
 -0.1158972692722755  3.1130004061531822 14.6032899135440317   T   T   T
  3.0723364177110080  3.0723364177110080 13.8569309599999944   F   F   F
  1.2028811542622144  4.6085046265665106 12.5708101129999950   F   F   F
  1.8526667528663046  4.5157099459514365 15.8168835638954537   T   T   T
  3.1684493990259068  3.0472901009859061 15.8768140671017814   T   T   T
  3.0951102669074415  4.6031550218652457 18.9305227064423356   T   T   T
  3.0107368279150526  2.9917099688641704 17.8037378330687872   T   T   T
  6.0961524415906760  3.0259029747121855 17.2534970270149302   T   T   T
  4.2366343414794336  4.6912209730919310 16.0051237836133176   T   T   T
  5.0266306726964478  4.8511144648670301 18.9012306798519170   T   T   T
 -0.3501753566545421  3.0817257468354455 19.2051522686403331   T   T   T
  3.8519093672953515  3.1312740222740012 20.1016112727516045   T   T   T
  1.1821111798611141  4.4077054702887226 19.4090544067900446   T   T   T
  0.3412924222939212  3.9630353734830277 23.8704844867463599   T   T   T
 -0.2624872450774253 -0.2878406061859806 21.8916446215445859   T   T   T
  1.5581645786835812  0.3131471883959540 23.9013973807128117   T   T   T
 -0.2723075648419727 -0.3233445843015029 25.8544376145882566   T   T   T
  0.9511337925939880  2.1256928873850538 21.7773127947167993   T   T   T
  2.7896140717873781  2.7543445418852892 23.8852775621247986   T   T   T
  0.9583710608657490  2.1387444756135086 25.8846543481544629   T   T   T
  2.1050428164715220  4.6070514512930432 21.9512635895556656   T   T   T
  4.0294062329608575  5.2153172666215433 23.9129535749918851   T   T   T
  2.1770706683688119  4.5841223910326239 25.8340362567909239   T   T   T
  3.4953351735242109  0.9701507939929584 21.9883141503808055   T   T   T
  5.2891150904160886  1.5395328585629555 23.9102706511275969   T   T   T
  3.4121044587176335  0.9192916531240931 25.8363489744800994   T   T   T
  4.7101694292761138  3.4260303737514883 21.9494518077879768   T   T   T
  4.6581633478231863  3.3673335118573369 25.8530406154111567   T   T   T

Oxide reference: TiO2(110)/fcc(100)_sqrt5/Pd E_tot= -422.16349459 eV
 D3-zero damping= -6.874447 eV, D3-BJ damping= -9.9984712 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
     6.1446728354220141    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1446728354220141    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.4848354988443120
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.5361682088555042  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.8694552634487942  1.5361682088555042  9.2861208469999994   F   F   F
  3.0723364177110080  0.0000000000000006  9.2861208469999994   F   F   F
  3.0723364177110080  1.5361682088555046 12.5708101129999967   F   F   F
```

```
  3.0723364177110080  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000006   F   F   F
  4.2752175719732213  1.5361682088555042  9.2861208469999994   F   F   F
  4.9417916811598008  1.5361682088555046 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000008 12.5708101129999967   F   F   F
  6.1446774883408679  1.5361682088555046 15.7086704500718124   T   T   T
  0.0000090843037081  0.0000000000000010 14.5675803801197610   T   T   T
  3.0723364177110080  0.0000000000000009 13.8569309599999961   F   F   F
  1.2028811542622142  1.5361682088555046 12.5708101129999967   F   F   F
  1.8617309673568692  1.5361682088555046 15.9066595067686105   T   T   T
  3.0723388862546521  0.0000000000000010 16.0586575925513024   T   T   T
  3.0723314358814187  1.5361682204842977 19.4752986489600985   T   T   T
  3.0723307193166227  0.0000000000000011 17.9059286125386556   T   T   T
  6.1446787786640114  0.0000000000000011 17.1105906247028869   T   T   T
  4.2829508612833775  1.5361682088555046 15.9066511313667096   T   T   T
  4.9896087882555147  1.5361682088555046 19.2718501601789356   T   T   T
 -0.0000110245118530  0.0000000000000012 18.9040720603592121   T   T   T
  3.0723580020922867  0.0000000000000013 20.5240625832172903   T   T   T
  1.1550595118672713  1.5361682088555046 19.2719096698989141   T   T   T
  0.0000000000000008  4.6085046265665106  9.2861208469999994   F   F   F
  0.0000000000000006  3.0723364177110080  8.0000000000000000   F   F   F
  1.8694552634487944  4.6085046265665106  9.2861208469999994   F   F   F
  3.0723364177110080  3.0723364177110080  9.2861208469999994   F   F   F
  3.0723364177110080  4.6085046265665106 12.5708101129999967   F   F   F
  3.0723364177110080  3.0723364177110080 11.2846892659999973   F   F   F
  0.0000000000000008  3.0723364177110080 10.5722416940000006   F   F   F
  4.2752175719732213  4.6085046265665106  9.2861208469999994   F   F   F
  4.9417916811598008  4.6085046265665106 12.5708101129999967   F   F   F
  0.0000000000000009  3.0723364177110080 12.5708101129999967   F   F   F
  6.1446774883408679  4.6085046265665106 15.7086704500718124   T   T   T
  0.0000090843037083  3.0723364177110080 14.5675803839307676   T   T   T
  3.0723364177110080  3.0723364177110080 13.8569309599999961   F   F   F
  1.2028811542622144  4.6085046265665106 12.5708101129999967   F   F   F
  1.8617309673568694  4.6085046265665106 15.9066595067686105   T   T   T
  3.0723388862546521  3.0723364177110080 16.0586575985987992   T   T   T
  3.0723314275814437  4.6085046149377291 19.4752986489600985   T   T   T
  3.0723307193166227  3.0723364177110080 17.9059286061525249   T   T   T
  6.1446787786640114  3.0723364177110080 17.1105906112439357   T   T   T
  4.2829508612833775  4.6085046265665106 15.9066511313667096   T   T   T
  4.9896087648786827  4.6085046265665115 19.2718501226439223   T   T   T
 -0.0000110245118529  3.0723364177110084 18.9040720639354838   T   T   T
  3.0723580020922867  3.0723364177110084 20.5240626231372900   T   T   T
  1.1550595012958620  4.6085046265665115 19.2719097297974180   T   T   T

Metal reference: TiO2(110)/fcc(100)_sqrt5/Pd E_tot= -76.1138396 eV
 D3-zero damping= -5.0956965 eV, D3-BJ damping= -6.2256799 eV
Pd
 1.0000000000000000
     6.1446728354220141    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1446728354220141    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9667868910931077
  15
Cartesian
  0.6142112562770361  4.3026567485211622 10.0128224803466743
 -0.0000000768461179 -0.0000046046186466  8.0552386615337834
  1.8423216788532180  0.6146996513856368 10.0128066621977094
  0.0000273926982794 -0.0000035621028497 11.9707745291220053
  1.2290907502328514  2.4578220496059293  8.0604931738222252
  3.0723460870632366  3.0723366754726147 10.0141674590950931
  1.2280688871970364  2.4571451231432881 11.9678722838797729
  2.4581458160346994  4.9160473732291319  8.0594281484814392
  4.3023751024846328  5.5299797237900714 10.0128027303909413
  2.4571662159003109  4.9162191922454550 11.9684127182965874
```

```
  3.6865291093579970  1.2286345873684033  8.0594328149979795
  5.5304910638103770  1.8420449643692527 10.0128362914109736
  3.6875420249991158  1.2284535324198527 11.9684295291401011
  4.9155656636578149  3.6868402711951762  8.0604865500001264
  4.9165971104558004  3.6875419563712875 11.9678748938731463

Interface: TiO2(110)/fcc(100)_sqrt5/Ir E_tot= -551.40728604 eV
 D3-zero damping= -16.2063377 eV, D3-BJ damping= -19.5509097 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ir
 1.0000000000000000
     6.0710659109428979    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.0710659109428979    0.0000000000000000
     0.0000000000000000    0.0000000000000000   33.8234733387352691
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000006  1.5177664777357252  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.8470610927452682  1.5177664777357252  9.2861208469999994   F   F   F
  3.0355329554714499  0.0000000000000006  9.2861208469999994   F   F   F
  3.0355329554714499  1.5177664777357256 12.5708101129999967   F   F   F
  3.0355329554714499  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000024   F   F   F
  4.2240048181976313  1.5177664777357252  9.2861208469999994   F   F   F
  4.8825940482167169  1.5177664777357256 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000008 12.5708101129999967   F   F   F
  6.0802210011340554  1.3512686899394590 16.0149442279871508   T   T   T
  0.0749746615242278 -0.0578060084401055 14.5771789424145091   T   T   T
  3.0355329554714499  0.0000000000000009 13.8569309599999961   F   F   F
  1.1884718627261825  1.5177664777357256 12.5708101129999967   F   F   F
  1.8551151317492853  1.6726268068891030 15.7592223090222969   T   T   T
  2.8013290967114401  0.0254628708752507 15.8374829304208653   T   T   T
  3.0812481103434957  1.5707102566204723 19.3396938209271667   T   T   T
  2.8476142963008768  0.1767418846876347 17.8154081674815927   T   T   T
  6.2509321416795744 -0.0220773705069540 17.1542241437606400   T   T   T
  4.2067092300218798  1.3784056543520145 15.8184187897634221   T   T   T
  4.9527046491179458  1.3117493368447708 19.2777267343905230   T   T   T
  0.2694524884055388 -0.1173265735605043 19.7632265460149696   T   T   T
  2.7954923134464158 -0.1293895875445582 20.2104329946403745   T   T   T
  1.1287419873462841  1.7252980421893165 19.8885880508684281   T   T   T
  0.0000000000000008  4.5532994332071741  9.2861208469999994   F   F   F
  0.0000000000000006  3.0355329554714499  8.0000000000000000   F   F   F
  1.8470610927452684  4.5532994332071741  9.2861208469999994   F   F   F
  3.0355329554714499  3.0355329554714499  9.2861208469999994   F   F   F
  3.0355329554714499  4.5532994332071741 12.5708101129999967   F   F   F
  3.0355329554714499  3.0355329554714499 11.2846892659999973   F   F   F
  0.0000000000000008  3.0355329554714499 10.5722416940000024   F   F   F
  4.2240048181976313  4.5532994332071741  9.2861208469999994   F   F   F
  4.8825940482167169  4.5532994332071741 12.5708101129999967   F   F   F
  0.0000000000000009  3.0355329554714499 12.5708101129999967   F   F   F
  6.0752965782781105  4.5135355372556312 15.7645080831015729   T   T   T
 -0.1378827910506613  3.0795211836703409 14.5697408533592867   T   T   T
  3.0355329554714499  3.0355329554714499 13.8569309599999961   F   F   F
  1.1884718627261828  4.5532994332071741 12.5708101129999967   F   F   F
  1.8808318088875111  4.4044369837762583 15.9513061146840283   T   T   T
  3.2594422378032797  3.0190564847505819 15.7785864064493868   T   T   T
  3.0636761518694970  4.6143592604547967 18.7481794004206463   T   T   T
  3.1439669606914942  2.9047968061925959 17.8752468374243385   T   T   T
  6.0054196981163317  2.9364658048226238 17.2082796863582104   T   T   T
  4.2017982026524585  4.6659706800397185 16.0683074308642944   T   T   T
  4.9246062948148674  4.6896210254531692 19.1423887691127632   T   T   T
 -0.2062049775979582  3.0281624624092625 19.0323189513147142   T   T   T
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  3.2423577298598603  3.2668292703715927 20.4550382413598655   T   T   T
  1.1998790551144007  4.3270287721904461 19.1776177581228779   T   T   T
  0.2511398260503511  3.3563177152565173 23.9344178914716323   T   T   T
 -0.3222184793635696 -0.8535799330928379 22.0642993636627764   T   T   T
  1.4690146862466955 -0.2689404868077783 23.9244554534394460   T   T   T
 -0.3296083673904625 -0.8708718127414430 25.7823793617373873   T   T   T
  0.8552150699709223  1.5876362339426622 22.0135834362773757   T   T   T
  2.6782823822705257  2.1508581951302586 23.9814763739836607   T   T   T
  0.8556336523435101  1.5354299309495170 25.8040740761935830   T   T   T
  2.0736472336946568  3.9577862941617621 22.1248639110237875   T   T   T
  3.9118952573628167  4.5909933089049293 23.9928247755093871   T   T   T
  2.0670623719076815  3.9904802726298878 25.8104654481965312   T   T   T
  3.3127370661242335  0.3238225416785186 22.0875169318639486   T   T   T
  5.1152235939095725  0.9661075372361233 23.9020894257363565   T   T   T
  3.2974909906015371  0.3367479577678331 25.7887078904205431   T   T   T
  4.5343243286757886  2.8081346692913645 22.0424547305905101   T   T   T
  4.5115163365618027  2.7548702283588455 25.7987807225625581   T   T   T

Oxide reference: TiO2(110)/fcc(100)_sqrt5/Ir E_tot= -421.09572473 eV
 D3-zero damping= -6.9907976 eV, D3-BJ damping= -10.1817933 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
     6.0710659109428979    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.0710659109428979    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.4848354988443120
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.5177664777357252  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.8470610927452682  1.5177664777357252  9.2861208469999994   F   F   F
  3.0355329554714499  0.0000000000000006  9.2861208469999994   F   F   F
  3.0355329554714499  1.5177664777357256 12.5708101129999967   F   F   F
  3.0355329554714499  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000006   F   F   F
  4.2240048181976313  1.5177664777357252  9.2861208469999994   F   F   F
  4.8825940482167169  1.5177664777357256 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000008 12.5708101129999967   F   F   F
  6.0710840428542134  1.5177664777357256 15.7139199673701260   T   T   T
  0.0000090070683899  0.0000000000000010 14.5746428607355334   T   T   T
  3.0355329554714499  0.0000000000000009 13.8569309599999961   F   F   F
  1.1884718627261825  1.5177664777357256 12.5708101129999967   F   F   F
  1.8419265573487833  1.5177664777357256 15.9575973408210956   T   T   T
  3.0355444658099460  0.0000000000000010 16.1507508927783867   T   T   T
  3.0355072243919099  1.5177664896903915 19.5914029614930243   T   T   T
  3.0354812319275508  0.0000000000000011 17.9930803190543358   T   T   T
  6.0711051867526402  0.0000000000000011 17.1377333453903944   T   T   T
  4.2291722637825675  1.5177664777357256 15.9576225254300486   T   T   T
  4.9270649548513648  1.5177664879925963 19.3338295099908422   T   T   T
 -0.0000036388995095  0.0000000000000012 18.9275576001274466   T   T   T
  3.0355914701402256  0.0000000000000013 20.6552790362857763   T   T   T
  1.1439604085965724  1.5177664777357256 19.3340242056861840   T   T   T
  0.0000000000000008  4.5532994332071741  9.2861208469999994   F   F   F
  0.0000000000000006  3.0355329554714499  8.0000000000000000   F   F   F
  1.8470610927452684  4.5532994332071741  9.2861208469999994   F   F   F
  3.0355329554714499  3.0355329554714499  9.2861208469999994   F   F   F
  3.0355329554714499  4.5532994332071741 12.5708101129999967   F   F   F
  3.0355329554714499  3.0355329554714499 11.2846892659999973   F   F   F
  0.0000000000000008  3.0355329554714499 10.5722416940000006   F   F   F
  4.2240048181976313  4.5532994332071741  9.2861208469999994   F   F   F
  4.8825940482167169  4.5532994332071741 12.5708101129999967   F   F   F
  0.0000000000000009  3.0355329554714499 12.5708101129999967   F   F   F
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  6.0710840662444365  4.5532994332071741 15.7139199745506524   T   T   T
  0.0000090070683901  3.0355329554714499 14.5746428607355334   T   T   T
  3.0355329554714499  3.0355329554714499 13.8569309599999961   F   F   F
  1.1884718627261828  4.5532994332071741 12.5708101129999967   F   F   F
  1.8419265761596451  4.5532994332071741 15.9575973360767414   T   T   T
  3.0355444960261191  3.0355329554714499 16.1507509441792401   T   T   T
  3.0355072174765607  4.5532994212525058 19.5914029614930243   T   T   T
  3.0354812319275508  3.0355329554714499 17.9930803437261773   T   T   T
  6.0711052169688129  3.0355329554714499 17.1377333141097061   T   T   T
  4.2291722561005880  4.5532994332071741 15.9576223976962943   T   T   T
  4.9270649510592248  4.5532994229503041 19.3338295413470682   T   T   T
 -0.0000035101773644  3.0355329554714503 18.9275575815691610   T   T   T
  3.0355914701402256  3.0355329554714503 20.6552791069748878   T   T   T
  1.1439603852311715  4.5532994332071750 19.3340242369477160   T   T   T

Metal reference: TiO2(110)/fcc(100)_sqrt5/Ir E_tot= -125.69073619 eV
 D3-zero damping= -6.2060759 eV, D3-BJ damping= -6.7262451 eV
Ir
 1.0000000000000000
     6.0710659109428979    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.0710659109428979    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9667868910931077
  15
Cartesian
  0.6071658439292177  4.2498534569187898 10.0137328163625625
  0.0000068174068811  0.0000026184530585  8.1624829936750221
  1.8211398775050429  0.6072651858802427 10.0135392332702526
  0.0000067829707242  0.0000026385922790 11.8646540304320052
  1.2142060955901579  2.4283091330655120  8.1626726654499908
  3.0355397975890734  3.0355355481809561 10.0133756213786498
  1.2141229680773027  2.4284485073587105 11.8645674966726276
  2.4284612053342003  4.8569122631033501  8.1626386859057973
  4.2499397988620125  5.4638061680487668 10.0135392421987905
  2.4286649576252621  4.8569243592683620 11.8645320424686709
  3.6426184597654601  1.2141590025361155  8.1626386608727941
  5.4639138635844438  1.8212178006420703 10.0137328273824338
  3.6424146472825329  1.2141469219919523 11.8645320416121276
  4.8568735751082119  3.6427620428013521  8.1626727170491886
  4.8569566294861071  3.6426226389465359 11.8645675820394167

Interface: TiO2(110)/fcc(100)_sqrt5/Rh E_tot= -527.18234565 eV
 D3-zero damping= -15.2843715 eV, D3-BJ damping= -18.9463148 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Rh
 1.0000000000000000
     5.9874358074613863    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.9874358074613863    0.0000000000000000
     0.0000000000000000    0.0000000000000000   33.8699998144521004
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000006  1.4968589518653472  9.2861208469999994   F   F   F
  0.0000000000000004  0.0000000000000005  7.9999999999999991   F   F   F
  1.8216174700620531  1.4968589518653472  9.2861208469999994   F   F   F
  2.9937179037306940  0.0000000000000006  9.2861208469999994   F   F   F
  2.9937179037306940  1.4968589518653477 12.5708101129999967   F   F   F
  2.9937179037306940  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000024   F   F   F
  4.1658183373993349  1.4968589518653472  9.2861208469999994   F   F   F
  4.8153353737927462  1.4968589518653477 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000008 12.5708101129999967   F   F   F
  5.9808839700266132  1.4342251933680903 16.1204790347367428   T   T   T
 -0.1723265573189907 -0.0178598695639511 14.5674266566138488   T   T   T
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  2.9937179037306940  0.0000000000000009 13.8569309599999961   F   F   F
  1.1721004336686418  1.4968589518653477 12.5708101129999967   F   F   F
  1.8183270512553229  1.3564286145394868 15.7354616261035218   T   T   T
  3.2137612292544806  0.0032318800095829 15.8171778229928179   T   T   T
  3.0410230703192469  1.4938482323562092 19.2752613749543613   T   T   T
  2.8994266256595420  0.1133856677940826 17.8379098717375868   T   T   T
  5.9859528887802345 -0.0387012321397812 17.1383208174152557   T   T   T
  4.1395082807769734  1.6386317661673042 15.8474761316826562   T   T   T
  4.9291162301259215  1.2286031574483958 19.2929323965264174   T   T   T
  0.3241895073317917 -0.0552340209322474 19.9180377283933261   T   T   T
  2.6980527078282619 -0.1091333750452135 20.3499958405969288   T   T   T
  1.1495716157599893  1.7894181045983493 19.9838731163347667   T   T   T
  0.0000000000000008  4.4905768555960401  9.2861208469999994   F   F   F
  0.0000000000000006  2.9937179037306940  7.9999999999999991   F   F   F
  1.8216174700620533  4.4905768555960401  9.2861208469999994   F   F   F
  2.9937179037306940  2.9937179037306940  9.2861208469999994   F   F   F
  2.9937179037306940  4.4905768555960401 12.5708101129999967   F   F   F
  2.9937179037306940  2.9937179037306940 11.2846892659999973   F   F   F
  0.0000000000000008  2.9937179037306940 10.5722416940000024   F   F   F
  4.1658183373993349  4.4905768555960401  9.2861208469999994   F   F   F
  4.8153353737927462  4.4905768555960401 12.5708101129999967   F   F   F
  0.0000000000000009  2.9937179037306940 12.5708101129999967   F   F   F
  5.9624970917290048  4.5223920390492331 15.7442277669587902   T   T   T
  0.0787008946785176  3.0215888510664932 14.5811002207423641   T   T   T
  2.9937179037306940  2.9937179037306940 13.8569309599999961   F   F   F
  1.1721004336686420  4.4905768555960401 12.5708101129999967   F   F   F
  1.8373198632731023  4.6041417599262360 15.9107009521011253   T   T   T
  2.7522281119925025  2.9734730245651644 15.7881401093565721   T   T   T
  3.0295380931599492  4.5155529958083864 18.8933600569074898   T   T   T
  2.8641392429261612  2.8888282064204560 17.8766185888766103   T   T   T
  6.0400782021952573  2.9247603184790893 17.3408031489905312   T   T   T
  4.1260182755459152  4.3442943879327069 16.0726710097424217   T   T   T
  4.9156677654882968  4.7790301352156064 19.1339943646638773   T   T   T
 -0.3018369641283381  3.0153953514563141 19.1831649029811260   T   T   T
  3.7142145347297726  3.0948924615165474 20.2298651027813605   T   T   T
  1.1969158489866751  4.2354429998960947 19.5201484010138593   T   T   T
  0.2271148602572172  3.6081017905486905 23.9870859323353365   T   T   T
 -0.3594111365749134 -0.5428428514551379 22.1700644349821481   T   T   T
  1.4207596669762539  0.0451168022118279 24.0118233229183708   T   T   T
 -0.3667388289322680 -0.5653873613349182 25.8327623079643054   T   T   T
  0.8461511648679239  1.8658092427444464 22.0824515691351131   T   T   T
  2.6180670803348498  2.4290656352040267 24.0139857574526054   T   T   T
  0.8244748461083479  1.8265787086248269 25.8454738649351370   T   T   T
  2.0148376842891871  4.2271412008339722 22.1756324762780928   T   T   T
  3.8173370389874126  4.8177978790596789 24.0347470086742199   T   T   T
  2.0155872977052995  4.2333647083742454 25.8626105922130165   T   T   T
  3.2564694576406739  0.6301459353330832 22.1695070915808650   T   T   T
  5.0202363456847126  1.2542427492671384 23.9757938231335928   T   T   T
  3.2229568252459537  0.6384201917751047 25.8371855983575038   T   T   T
  4.4125995617455533  3.0531371850296707 22.1362952708808578   T   T   T
  4.4267477781869262  3.0251049856371361 25.8344935162492071   T   T   T

Oxide reference: TiO2(110)/fcc(100)_sqrt5/Rh E_tot= -419.12732285 eV
 D3-zero damping= -7.0917166 eV, D3-BJ damping= -10.3403587 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
     5.9874358074613863    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.9874358074613863    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.4848354988443120
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
```

```
  0.0000000000000006  1.4968589518653472  9.2861208469999994   F   F   F
  0.0000000000000004  0.0000000000000005  8.0000000000000000   F   F   F
  1.8216174700620531  1.4968589518653472  9.2861208469999994   F   F   F
  2.9937179037306940  0.0000000000000006  9.2861208469999994   F   F   F
  2.9937179037306940  1.4968589518653477 12.5708101129999967   F   F   F
  2.9937179037306940  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000006   F   F   F
  4.1658183373993349  1.4968589518653472  9.2861208469999994   F   F   F
  4.8153353737927462  1.4968589518653477 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000008 12.5708101129999967   F   F   F
  5.9874523466492056  1.4968589518653477 15.7399006081770594   T   T   T
  0.0000026382171125  0.0000000000000008 14.6030283439469795   T   T   T
  2.9937179037306940  0.0000000000000009 13.8569309599999961   F   F   F
  1.1721004336686418  1.4968589518653477 12.5708101129999967   F   F   F
  1.8186165252026736  1.4968588735302562 16.0711022408248319   T   T   T
  2.9937303199907732  0.0000000000000011 16.3474635042287879   T   T   T
  2.9937734901976625  1.4968589337246698 19.8071726826972494   T   T   T
  2.9936760116538457  0.0000000000000011 18.1741443734488684   T   T   T
  5.9874659421733458  0.0000000000000011 17.2083321672923830   T   T   T
  4.1688520283279713  1.4968590587671398 16.0711086788598330   T   T   T
  4.8537373844738534  1.4968589518653477 19.4580106175928051   T   T   T
  0.0000820055772686  0.0000000000000012 18.9941740430412338   T   T   T
  2.9937926613647123  0.0000000000000013 20.8853449642088087   T   T   T
  1.1337565791732898  1.4968589518653477 19.4582122870093919   T   T   T
  0.0000000000000008  4.4905768555960401  9.2861208469999994   F   F   F
  0.0000000000000006  2.9937179037306940  8.0000000000000000   F   F   F
  1.8216174700620533  4.4905768555960401  9.2861208469999994   F   F   F
  2.9937179037306940  2.9937179037306940  9.2861208469999994   F   F   F
  2.9937179037306940  4.4905768555960401 12.5708101129999967   F   F   F
  2.9937179037306940  2.9937179037306940 11.2846892659999973   F   F   F
  0.0000000000000008  2.9937179037306940 10.5722416940000006   F   F   F
  4.1658183373993349  4.4905768555960401  9.2861208469999994   F   F   F
  4.8153353737927462  4.4905768555960401 12.5708101129999967   F   F   F
  0.0000000000000009  2.9937179037306940 12.5708101129999967   F   F   F
  5.9874523466492056  4.4905768555960401 15.7399005997274326   T   T   T
  0.0000027037298946  2.9937179037306940 14.6030283436320278   T   T   T
  2.9937179037306940  2.9937179037306940 13.8569309599999961   F   F   F
  1.1721004336686420  4.4905768555960401 12.5708101129999967   F   F   F
  1.8186165252026738  4.4905769339311394 16.0711022408248319   T   T   T
  2.9937300679515593  2.9937179037306940 16.3474635357918636   T   T   T
  2.9937734799999274  4.4905768737367273 19.8071726826972494   T   T   T
  2.9936759691442107  2.9937179037306940 18.1741443734896926   T   T   T
  5.9874660868551972  2.9937179037306940 17.2083321682406272   T   T   T
  4.1688520283279713  4.4905767844726450 16.0711087003956408   T   T   T
  4.8537373905020651  4.4905768555960410 19.4580106175928051   T   T   T
  0.0000820055772688  2.9937179037306945 18.9941740437719666   T   T   T
  2.9937926421226444  2.9937179037306945 20.8853449152449251   T   T   T
  1.1337565851907099  4.4905768555960410 19.4582122641026878   T   T   T

Metal reference: TiO2(110)/fcc(100)_sqrt5/Rh E_tot= -103.52099983 eV
 D3-zero damping= -5.0103315 eV, D3-BJ damping= -6.042363 eV
Rh
 1.0000000000000000
     5.9874358074613863    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.9874358074613863    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9667868910931077
  15
Cartesian
  0.5991460472901498  4.1907757726851242 10.0150635080725596
  0.0000198652003520 -0.0000117842383160  8.1720154008921266
  1.7949921946917182  0.5981710476730787 10.0107669427260220
  0.0000072241854641  0.0000237723263443 11.8563600781859844
  1.1957245128519236  2.3957929000964104  8.1721006331294159
```

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  2.9937219546542089  2.9937247149562753 10.0122360032175326
  1.1984605335984095  2.3940155168809034 11.8556348545542871
  2.3953737281868785  4.7900643314578719  8.1728125625069605
  4.1924601591514579  5.3892701241284833 10.0107660373601881
  2.3967947350967487  4.7906345779471717 11.8553088482271285
  3.5920567184454177  1.1973682119152573  8.1727935023086857
  5.3882867563422883  1.7966618067602611 10.0149800125014572
  3.5906713935645196  1.1968098056155676 11.8553048992869883
  4.7917394814709580  3.5916705651964920  8.1720901452138008
  4.7889792104556044  3.5934005988106184 11.8556452442286311

Interface: TiO2(110)/fcc(100)_sqrt5/Os E_tot= -579.97977282 eV
 D3-zero damping= -14.0188011 eV, D3-BJ damping= -18.5157482 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Os
 1.0000000000000000
     6.0561984481982405    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.0561984481982405    0.0000000000000000
     0.0000000000000000    0.0000000000000000   33.8656064257491494
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000006  1.5140496120495608  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.8425378158798336  1.5140496120495608  9.2861208469999994   F   F   F
  3.0280992240991211  0.0000000000000006  9.2861208469999994   F   F   F
  3.0280992240991211  1.5140496120495612 12.5708101129999967   F   F   F
  3.0280992240991211  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000024   F   F   F
  4.2136606323184083  1.5140496120495608  9.2861208469999994   F   F   F
  4.8706370399789529  1.5140496120495612 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000008 12.5708101129999967   F   F   F
  6.0702938505978628  1.3497343023517447 16.0144368216497810   T   T   T
  0.0694462988641865 -0.0570069745491026 14.5746147943028266   T   T   T
  3.0280992240991211  0.0000000000000009 13.8569309599999961   F   F   F
  1.1855614082192882  1.5140496120495612 12.5708101129999967   F   F   F
  1.8558588589661738  1.6736286422546336 15.7493501267670766   T   T   T
  2.7876989176394131  0.0258231084626980 15.8373985509063235   T   T   T
  3.0885515574540259  1.5625713421235725 19.3397501089412884   T   T   T
  2.8259837927213405  0.1833042178554785 17.8384819790367857   T   T   T
  6.2562834297242720 -0.0309729716730960 17.1425924309876336   T   T   T
  4.1972396344473815  1.3669342942703187 15.8433016365743420   T   T   T
  4.9604414057319648  1.3188810186637849 19.2820891591446113   T   T   T
  0.2526450481451143 -0.1407977775137026 19.8247590911346805   T   T   T
  2.9280927359669686 -0.1428488424175691 20.2690641375340448   T   T   T
  1.1572338893630103  1.6874469795680613 19.9608113476790088   T   T   T
  0.0000000000000008  4.5421488361486801  9.2861208469999994   F   F   F
  0.0000000000000006  3.0280992240991211  8.0000000000000000   F   F   F
  1.8425378158798338  4.5421488361486801  9.2861208469999994   F   F   F
  3.0280992240991211  3.0280992240991211  9.2861208469999994   F   F   F
  3.0280992240991211  4.5421488361486801 12.5708101129999967   F   F   F
  3.0280992240991211  3.0280992240991211 11.2846892659999973   F   F   F
  0.0000000000000008  3.0280992240991211 10.5722416940000024   F   F   F
  4.2136606323184083  4.5421488361486801  9.2861208469999994   F   F   F
  4.8706370399789529  4.5421488361486801 12.5708101129999967   F   F   F
  0.0000000000000009  3.0280992240991211 12.5708101129999967   F   F   F
  6.0608034588231465  4.5057802652222305 15.7695574993207046   T   T   T
 -0.1602390146106338  3.0676997445937246 14.5764135358901648   T   T   T
  3.0280992240991211  3.0280992240991211 13.8569309599999961   F   F   F
  1.1855614082192885  4.5421488361486801 12.5708101129999967   F   F   F
  1.8814247219782394  4.3884258220071182 15.9318614791142128   T   T   T
  3.2655891738567204  3.0145785046587763 15.7756348868764782   T   T   T
  3.0742451815482630  4.6115187937649473 18.7616868040786962   T   T   T
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  3.1228175536888263  2.8991267029465710 17.8874858886735133   T   T   T
  6.0229328253939345  2.9288975803993735 17.2163319736436620   T   T   T
  4.1928279876730503  4.6604807901774352 16.1040052117145045   T   T   T
  4.9386234507907760  4.6399370701638745 19.1370349482490738   T   T   T
 -0.1523201211212120  3.0037188804425354 19.0416110112078876   T   T   T
  3.2628425311183427  3.2560132328377094 20.5124001324056771   T   T   T
  1.2366451468511157  4.3147546681769899 19.2484646249363749   T   T   T
  0.3236765474500273  3.3337241021520767 23.9878945316352237   T   T   T
 -0.2801151423357274 -0.8724246217101125 22.1270289275636891   T   T   T
  1.5408497503519960 -0.1975554566003292 23.8883614677505278   T   T   T
 -0.2517180237955642 -0.7963540601092998 25.8138407278411215   T   T   T
  0.8922125425191572  1.6235097311260589 22.0576918854908541   T   T   T
  2.7348163661669185  2.1507022148061958 23.9115367601838251   T   T   T
  0.9437988668292023  1.6032931446423195 25.8291814420557166   T   T   T
  2.1336410527754830  3.9844404250673771 22.1723961027564123   T   T   T
  3.8643002190316378  4.5760424136542541 24.1993608891701726   T   T   T
  2.0033753677160431  4.0154893443080155 25.8841352644149367   T   T   T
  3.3881007042635094  0.3021990312155467 22.1444637225682932   T   T   T
  5.1598088300850646  1.0113896385046908 23.8817727864922880   T   T   T
  3.3274147516425203  0.4491130228155829 25.8641708081723003   T   T   T
  4.5599072061644526  2.9194845355324146 22.1069214887850300   T   T   T
  4.6122264427554196  2.6901483106392003 25.8769020876277906   T   T   T

Oxide reference: TiO2(110)/fcc(100)_sqrt5/Os E_tot= -420.80564609 eV
 D3-zero damping= -7.0127133 eV, D3-BJ damping= -10.2160606 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
     6.0561984481982405    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.0561984481982405    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.4848354988443120
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.5140496120495608  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  1.8425378158798336  1.5140496120495608  9.2861208469999994   F   F   F
  3.0280992240991211  0.0000000000000006  9.2861208469999994   F   F   F
  3.0280992240991211  1.5140496120495612 12.5708101129999967   F   F   F
  3.0280992240991211  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000006   F   F   F
  4.2136606323184083  1.5140496120495608  9.2861208469999994   F   F   F
  4.8706370399789529  1.5140496120495612 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000008 12.5708101129999967   F   F   F
  6.0562099454778169  1.5140496120495612 15.7175004550971060   T   T   T
  0.0000049989267150  0.0000000000000008 14.5781998497335561   T   T   T
  3.0280992240991211  0.0000000000000009 13.8569309599999961   F   F   F
  1.1855614082192882  1.5140496120495612 12.5708101129999967   F   F   F
  1.8379723264993424  1.5140496120495612 15.9711982170387827   T   T   T
  3.0281053254527794  0.0000000000000009 16.1746593955256728   T   T   T
  3.0281170242933180  1.5140496130566727 19.6188205198935925   T   T   T
  3.0280516187477087  0.0000000000000011 18.0148980851866654   T   T   T
  6.0562270218931058  0.0000000000000011 17.1470737938735454   T   T   T
  4.2182485213349574  1.5140496120495612 15.9712088929757758   T   T   T
  4.9144070440544532  1.5140496120495612 19.3504681664294758   T   T   T
  0.0000359438665423  0.0000000000000012 18.9362496327233458   T   T   T
  3.0281599815907807  0.0000000000000013 20.6852940464935173   T   T   T
  1.1417933840208567  1.5140496120495612 19.3506550343868042   T   T   T
  0.0000000000000008  4.5421488361486801  9.2861208469999994   F   F   F
  0.0000000000000006  3.0280992240991211  8.0000000000000000   F   F   F
  1.8425378158798338  4.5421488361486801  9.2861208469999994   F   F   F
  3.0280992240991211  3.0280992240991211  9.2861208469999994   F   F   F
  3.0280992240991211  4.5421488361486801 12.5708101129999967   F   F   F
```

```
  3.0280992240991211  3.0280992240991211 11.2846892659999973   F   F   F
  0.0000000000000008  3.0280992240991211 10.5722416940000006   F   F   F
  4.2136606323184083  4.5421488361486801  9.2861208469999994   F   F   F
  4.8706370399789529  4.5421488361486801 12.5708101129999967   F   F   F
  0.0000000000000009  3.0280992240991211 12.5708101129999967   F   F   F
  6.0562099454778169  4.5421488361486801 15.7175004550971060   T   T   T
  0.0000049989267153  3.0280992240991211 14.5781998442358507   T   T   T
  3.0280992240991211  3.0280992240991211 13.8569309599999961   F   F   F
  1.1855614082192885  4.5421488361486801 12.5708101129999967   F   F   F
  1.8379723264993428  4.5421488361486801 15.9711982170387827   T   T   T
  3.0281053254527794  3.0280992240991211 16.1746594032559479   T   T   T
  3.0281170407401916  4.5421488351415658 19.6188205198935925   T   T   T
  3.0280516187477087  3.0280992240991211 18.0148981043037182   T   T   T
  6.0562270218931058  3.0280992240991211 17.1470737828454745   T   T   T
  4.2182485213349574  4.5421488361486801 15.9712088929757758   T   T   T
  4.9144070605269707  4.5421488361486810 19.3504681664294758   T   T   T
  0.0000359438665425  3.0280992240991216 18.9362496156779656   T   T   T
  3.0281599815907807  3.0280992240991216 20.6852940756320507   T   T   T
  1.1417933840208569  4.5421488361486810 19.3506550343868184   T   T   T

Metal reference: TiO2(110)/fcc(100)_sqrt5/Os E_tot= -154.45866214 eV
 D3-zero damping= -4.818389 eV, D3-BJ damping= -5.7754718 eV
Os
 1.0000000000000000
     6.0561984481982405    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.0561984481982405    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9667868910931077
  15
Cartesian
  0.6053802669408869  4.2395530549122311 10.0100973182017974
 -0.0000007105213299  0.0000021011675965  8.1622286309141483
  1.8168744796835901  0.6057587409888333 10.0187844596680335
  0.0000157930269510  0.0000033144599225 11.8646992256756043
  1.2120522394904123  2.4208463401024600  8.1613193404906532
  3.0281071412258194  3.0281022066371026 10.0107208562558316
  1.2099350540305427  2.4250589782170344 11.8647598889757440
  2.4232216007947085  4.8479009764557786  8.1626589990144378
  4.2393409793725523  5.4504451076136684 10.0188093114359091
  2.4217236848556043  4.8420115205136653 11.8654686634384490
  3.6330035782605874  1.2083026511297907  8.1626601474350320
  5.4508335573726354  1.8166512809800353 10.0101095928285666
  3.6344774653153618  1.2141935813773073 11.8654698204271121
  4.8441559873073023  3.6353587849883211  8.1613223406832258
  4.8462716391569298  3.6311408638907614 11.8647695749891842

Interface: TiO2(110)/fcc(100)_sqrt5/Ru E_tot= -553.20238564 eV
 D3-zero damping= -14.8631476 eV, D3-BJ damping= -18.3607363 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ru
 1.0000000000000000
     5.9617926842303506    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.9617926842303506    0.0000000000000000
     0.0000000000000000    0.0000000000000000   33.7524284002377044
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000006  1.4904481710575881  9.2861208469999994   F   F   F
  0.0000000000000004  0.0000000000000005  7.9999999999999991   F   F   F
  1.8138158062502425  1.4904481710575881  9.2861208469999994   F   F   F
  2.9808963421151762  0.0000000000000006  9.2861208469999994   F   F   F
  2.9808963421151762  1.4904481710575885 12.5708101129999967   F   F   F
  2.9808963421151762  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416939999988   F   F   F
```

```
  4.1479768779801089  1.4904481710575881  9.2861208469999994   F   F   F
  4.7947121483654174  1.4904481710575885 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000008 12.5708101129999967   F   F   F
  5.8780196444203954  1.4541711626916087 15.9536194239435662   T   T   T
  0.0453500976077952  0.0172749466544883 14.6393581535678354   T   T   T
  2.9808963421151762  0.0000000000000009 13.8569309599999961   F   F   F
  1.1670805358649341  1.4904481710575885 12.5708101129999967   F   F   F
  1.7633263497261045  1.3912202241734626 16.4866568170194014   T   T   T
  3.2626029206062030 -0.0311173996173164 16.5229610296885987   T   T   T
  2.6765158586612721  1.4909434059071132 19.3880566644761387   T   T   T
  3.0689347263293101 -0.0985104472219216 18.3972470259408816   T   T   T
  5.3309528302929978 -0.0061604288085171 17.1268320345385376   T   T   T
  3.9848333117906733  1.6495613362762123 15.8457635098061331   T   T   T
  4.5288584770387832  1.4689332167725933 20.2835190595336776   T   T   T
  0.0415291952723677  0.0752425986888152 20.3703474963240936   T   T   T
  2.1357251567281268  0.1234072856304137 20.7237632223485839   T   T   T
  0.7641969538264550  1.5725826421852824 19.2351050694144909   T   T   T
  0.0000000000000008  4.4713445131727623  9.2861208469999994   F   F   F
  0.0000000000000006  2.9808963421151762  7.9999999999999991   F   F   F
  1.8138158062502427  4.4713445131727623  9.2861208469999994   F   F   F
  2.9808963421151762  2.9808963421151762  9.2861208469999994   F   F   F
  2.9808963421151762  4.4713445131727623 12.5708101129999967   F   F   F
  2.9808963421151762  2.9808963421151762 11.2846892659999973   F   F   F
  0.0000000000000008  2.9808963421151762 10.5722416939999988   F   F   F
  4.1479768779801089  4.4713445131727623  9.2861208469999994   F   F   F
  4.7947121483654174  4.4713445131727623 12.5708101129999967   F   F   F
  0.0000000000000009  2.9808963421151762 12.5708101129999967   F   F   F
  5.8705782793435279  4.5307807654989034 15.9849921254930383   T   T   T
  0.3935139164371478  2.9674359379310742 14.7588309211782907   T   T   T
  2.9808963421151762  2.9808963421151762 13.8569309599999961   F   F   F
  1.1670805358649343  4.4713445131727623 12.5708101129999967   F   F   F
  1.7712361645867043  4.5756591051523152 16.4078289028510618   T   T   T
  2.5425187169087811  2.9732136155497839 15.6495241455260476   T   T   T
  2.6690407399366376  4.3924859085838825 19.9342387569029214   T   T   T
  3.3973105856254997  3.0588553410429555 18.5944431505201955   T   T   T
  5.7180858678357964  3.0140182194090550 17.3205486156598276   T   T   T
  3.9937681258433715  4.2972289493791793 15.7889960321395115   T   T   T
  4.6139906467704934  4.5142776044547945 20.4272709068963962   T   T   T
 -0.5579244124600550  3.0055083459100227 19.1549918776489747   T   T   T
  2.4070953335715188  2.7435698926219865 20.9931624500401384   T   T   T
  0.8228127864314695  4.3593259420728590 19.4071396343279190   T   T   T
  0.6654994601439399  4.9155327950257650 24.3820498282115672   T   T   T
  0.0469890677409506  0.7902993596861203 22.6854940392581419   T   T   T
  1.9158870036614921  1.3942923391610793 24.4459470216134065   T   T   T
  0.0772688714209153  0.8113169812447012 26.2215075571760110   T   T   T
  1.1866279803346289  3.1393017141126678 22.5516947996086010   T   T   T
  3.0368007168544615  3.7453503724246899 24.3168994108242593   T   T   T
  1.2446593965158086  3.1820355783132226 26.2353910933384675   T   T   T
  2.4050398955429086  5.5874658907752632 22.6175856802001078   T   T   T
  4.1746682786835585  6.0944089511434818 24.3679784948172156   T   T   T
  2.4365004122224021  5.5723735608195337 26.2441712628382611   T   T   T
  3.7760081391810099  1.9467873984434574 22.4393530368837517   T   T   T
  5.3873464528238877  2.6737492792861404 24.4371926062944524   T   T   T
  3.6870401771475225  1.9225611412483865 26.2718653252001921   T   T   T
  4.8500618548378620  4.3508867573046475 22.5219007592999603   T   T   T
  4.7766168647400553  4.3423596358631880 26.2373702430579456   T   T   T

Oxide reference: TiO2(110)/fcc(100)_sqrt5/Ru E_tot= -418.37040121 eV
 D3-zero damping= -7.1232548 eV, D3-BJ damping= -10.3921199 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
     5.9617926842303506    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.9617926842303506    0.0000000000000000
```

```
     0.0000000000000000    0.0000000000000000   28.4848354988443120
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.4904481710575881  9.2861208469999994   F   F   F
  0.0000000000000004  0.0000000000000005  8.0000000000000000   F   F   F
  1.8138158062502425  1.4904481710575881  9.2861208469999994   F   F   F
  2.9808963421151762  0.0000000000000006  9.2861208469999994   F   F   F
  2.9808963421151762  1.4904481710575885 12.5708101129999967   F   F   F
  2.9808963421151762  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000007 10.5722416940000006   F   F   F
  4.1479768779801089  1.4904481710575881  9.2861208469999994   F   F   F
  4.7947121483654174  1.4904481710575885 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000008 12.5708101129999967   F   F   F
  5.9617975607000702  1.4904481703645593 15.7482232214208917   T   T   T
  0.0000088145063371  0.0000000000000017 14.6107414187029843   T   T   T
  2.9808963421151762  0.0000000000000009 13.8569309599999961   F   F   F
  1.1670805358649341  1.4904481710575885 12.5708101129999967   F   F   F
  1.8115804338507340  1.4904483340451882 16.1034664142298531   T   T   T
  2.9808977387263518 -0.0000000271385201 16.4071669800712669   T   T   T
  2.9809424483234328  1.4904482441730669 19.8698756912815178   T   T   T
  2.9808417135409524 -0.0000001017384280 18.2280600846144942   T   T   T
  5.9618008480566216  0.0000000000000010 17.2301058266747766   T   T   T
  4.1502176203933683  1.4904480111602521 16.1034443723993412   T   T   T
  4.8312481245184591  1.4904482567151205 19.4947537557631492   T   T   T
  0.0000729184318963  0.0000000201967332 19.0147537293394677   T   T   T
  2.9809756172368749  0.0000000619392024 20.9529525620116921   T   T   T
  1.1305785990105031  1.4904481710575885 19.4949642668315377   T   T   T
  0.0000000000000008  4.4713445131727623  9.2861208469999994   F   F   F
  0.0000000000000006  2.9808963421151762  8.0000000000000000   F   F   F
  1.8138158062502427  4.4713445131727623  9.2861208469999994   F   F   F
  2.9808963421151762  2.9808963421151762  9.2861208469999994   F   F   F
  2.9808963421151762  4.4713445131727623 12.5708101129999967   F   F   F
  2.9808963421151762  2.9808963421151762 11.2846892659999973   F   F   F
  0.0000000000000008  2.9808963421151762 10.5722416940000006   F   F   F
  4.1479768779801089  4.4713445131727623  9.2861208469999994   F   F   F
  4.7947121483654174  4.4713445131727623 12.5708101129999967   F   F   F
  0.0000000000000009  2.9808963421151762 12.5708101129999967   F   F   F
  5.9617975660183165  4.4713444914593845 15.7482232021332589   T   T   T
  0.0000086685303693  2.9808963173165224 14.6107414075649178   T   T   T
  2.9808963421151762  2.9808963421151762 13.8569309599999961   F   F   F
  1.1670805358649343  4.4713445131727623 12.5708101129999967   F   F   F
  1.8115804474292760  4.4713443377523276 16.1034663326881429   T   T   T
  2.9808982756693765  2.9808963421151762 16.4071670955299673   T   T   T
  2.9809424462959795  4.4713445918131978 19.8698756192415757   T   T   T
  2.9808416918015261  2.9808964175016261 18.2280601700457972   T   T   T
  5.9618005680947812  2.9808963421151762 17.2301057530332962   T   T   T
  4.1502176306644474  4.4713446467181219 16.1034443031746690   T   T   T
  4.8312481544389776  4.4713444860342424 19.4947539466346988   T   T   T
  0.0000730925100830  2.9808963638364099 19.0147536480918475   T   T   T
  2.9809755637923936  2.9808964067088755 20.9529525353317183   T   T   T
  1.1305785829937263  4.4713445379714152 19.4949642862282815   T   T   T

Metal reference: TiO2(110)/fcc(100)_sqrt5/Ru E_tot= -128.16130815 eV
 D3-zero damping= -4.7328002 eV, D3-BJ damping= -5.7729279 eV
Ru
 1.0000000000000000
     5.9617926842303506    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.9617926842303506    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9667868910931077
  15
Cartesian
```

```
  0.5975242314748939  4.1720329478522515 10.0420367194571156
 -0.0000560826471376 -0.0000668510180765  8.1830571402538883
  1.7884342297133757  0.5965638026764019 10.0060507790365634
  0.0002206789584744  0.0000180379967619 11.8440184530296406
  1.1692941008323856  2.3706935443782422  8.1836299437845295
  2.9809347014884282  2.9809566062910231  9.9747194613206158
  1.2144835616697722  2.3962631140644945 11.8444129293143732
  2.3696405611979947  4.7699627375470746  8.1811770046567407
  4.1737280356641602  5.3654162873601168 10.0060109273548132
  2.4029622297324873  4.7752775603834285 11.8434292957702976
  3.5918062390359862  1.1916402288540957  8.1813254750502757
  5.3641324856549470  1.7896732547313026 10.0424540124477595
  3.5586833108318174  1.1866285855102077 11.8435412551291002
  4.7926017109453571  3.5911346561375237  8.1836170558034596
  4.7473635893912398  3.5654968672766043 11.8443985235746627

Interface: TiO2(110)/fcc(100)_5x1/Au E_tot= -474.98577988 eV
 D3-zero damping= -15.3589248 eV, D3-BJ damping= -17.130843 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Au
 1.0000000000000000
    14.4937585523500019    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8987517104700005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.5836913096048377
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000007  1.4493758552350009  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  7.9999999999999991   F   F   F
  2.2047905509834833  1.4493758552350009  9.2861208469999994   F   F   F
  3.6234396380875014  0.0000000000000006  9.2861208469999994   F   F   F
  3.6234396380875014  1.4493758552350011 12.5708101129999967   F   F   F
  3.6234396380875014  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416939999988   F   F   F
  5.0420887251915198  1.4493758552350009  9.2861208469999994   F   F   F
  5.8282301890709833  1.4493758552350011 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000008 12.5708101129999967   F   F   F
 14.1349350020436280  1.4493758552350011 15.8350543037847267   T   T   T
 -0.0344482357592523  0.0000000000000017 14.6499955123282355   T   T   T
  3.6234396380875014  0.0000000000000008 13.8569309599999961   F   F   F
  1.4186490871040189  1.4493758552350011 12.5708101129999967   F   F   F
  2.2545304898070095  1.4493758552350011 15.8321105929037316   T   T   T
  3.4344765863606566  0.0000000000000016 15.8797848551877134   T   T   T
  3.1790980974309280  1.4493758552350018 19.1724741697516414   T   T   T
  3.4731838701960767  0.0000000000000002 17.8375229601143772   T   T   T
 14.4138706677580810  0.0000000000000008 17.2122546945377444   T   T   T
  4.9458052569148148  1.4493758552350011 15.8938837649645919   T   T   T
  6.3335535427003444  1.4493758552350018 19.5190995505584439   T   T   T
 -0.1239653759006191  0.0000000000000013 19.0841256193289261   T   T   T
  3.6121724139573481  0.0000000000000013 20.3028129645580258   T   T   T
  1.2826876184480571  1.4493758552350018 19.3121178726268674   T   T   T
  7.2468792761750027  1.4493758552350009  9.2861208469999994   F   F   F
  7.2468792761750027  0.0000000000000005  7.9999999999999991   F   F   F
  9.4516698271584829  1.4493758552350009  9.2861208469999994   F   F   F
 10.8703189142625032  0.0000000000000006  9.2861208469999994   F   F   F
 10.8703189142625032  1.4493758552350011 12.5708101129999967   F   F   F
 10.8703189142625032  0.0000000000000007 11.2846892659999973   F   F   F
  7.2468792761750027  0.0000000000000006 10.5722416939999988   F   F   F
 12.2889680013665199  1.4493758552350009  9.2861208469999994   F   F   F
 13.0751094652459869  1.4493758552350011 12.5708101129999967   F   F   F
  7.2468792761750027  0.0000000000000008 12.5708101129999967   F   F   F
  6.7830562849322886  1.4493758552350011 15.8559392202307112   T   T   T
  7.1524040187126019  0.0000000000000009 14.6715293072112232   T   T   T
```

```
 10.8703189142625032  0.0000000000000008 13.8569309599999961   F   F   F
  8.6655283632790212  1.4493758552350011 12.5708101129999967   F   F   F
  9.6309283461392958  1.4493758552350011 15.9219165318426068   T   T   T
 10.7967047384175387  0.0000000000000008 15.9172087691881021   T   T   T
 10.7687164095921695  1.4493758552350018 19.2169963568671029   T   T   T
 11.0043561861354284  0.0000000000000010 17.8835046958161854   T   T   T
  7.1362097096657759  0.0000000000000010 17.2033416499910672   T   T   T
 12.3025749716024890  1.4493758552350011 15.8457800242195823   T   T   T
 13.1835188503405938  1.4493758552350018 19.3397540765889246   T   T   T
  7.4216143940356636  0.0000000000000011 19.0726599404841366   T   T   T
 10.9435575926537574  0.0000000000000011 20.4627125004831214   T   T   T
  8.8566973463254470  1.4493758552350018 19.1681630370956668   T   T   T
  0.8189885369395958 -0.0000000000000001 22.2531623834809444   T   T   T
  2.1405083792776387  1.4493758552350002 24.5214599961966400   T   T   T
  0.6453399573651296 -0.0000000000000002 26.4886401336926980   T   T   T
  3.6118265599118438 -0.0000000000000000 22.5506496616167809   T   T   T
  5.0581798147413064  1.4493758552350002 24.5630107611107782   T   T   T
  3.5993768442483494 -0.0000000000000000 26.6414355384470127   T   T   T
  6.3996350204133190 -0.0000000000000000 22.3766834190590664   T   T   T
  7.9824897987160748  1.4493758552350002 24.3898224702931223   T   T   T
  6.5745113916875599  0.0000000000000001 26.5235062832707058   T   T   T
  9.1333818315857087  0.0000000000000001 22.1802987689960283   T   T   T
 10.8602543318769786  1.4493758552350002 24.0823777420966678   T   T   T
  9.4796120630692684  0.0000000000000001 26.3820299402380414   T   T   T
 12.5722477447984549  0.0000000000000000 22.1702944621525972   T   T   T
 13.7477270870488706  1.4493758552350002 24.3359611491300605   T   T   T
 12.2566926527132036  0.0000000000000000 26.3550115165031009   T   T   T

Oxide reference: TiO2(110)/fcc(100)_5x1/Au E_tot= -422.25357853 eV
 D3-zero damping= -6.4120302 eV, D3-BJ damping= -8.9369632 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
    14.4937585523500019    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8987517104700005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.4277616613406394
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000007  1.4493758552350009  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  2.2047905509834833  1.4493758552350009  9.2861208469999994   F   F   F
  3.6234396380875014  0.0000000000000006  9.2861208469999994   F   F   F
  3.6234396380875014  1.4493758552350011 12.5708101129999967   F   F   F
  3.6234396380875014  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416940000006   F   F   F
  5.0420887251915198  1.4493758552350009  9.2861208469999994   F   F   F
  5.8282301890709833  1.4493758552350011 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000008 12.5708101129999967   F   F   F
 14.0558096045795882  1.4493758552350011 15.8101015061887615   T   T   T
 -0.0795865511625414  0.0000000000000014 14.6290904546441496   T   T   T
  3.6234396380875014  0.0000000000000008 13.8569309599999961   F   F   F
  1.4186490871040189  1.4493758552350011 12.5708101129999967   F   F   F
  2.2914165297686448  1.4493758552350011 15.8753368451823693   T   T   T
  3.4573855704980967  0.0000000000000006 15.9944315672598147   T   T   T
  3.2933341721076781  1.4493758552350018 19.3227237920783566   T   T   T
  3.5648683791238129  0.0000000000000012 17.8929248569216490   T   T   T
 14.3909097753304120  0.0000000000000010 17.1594311584347743   T   T   T
  4.9824408214635616  1.4493758552350011 15.8774191478351874   T   T   T
  6.1513970549578918  1.4493758552350018 19.4419899860881564   T   T   T
 -0.0284807964610550  0.0000000000000012 19.0239088882035468   T   T   T
  3.5937687569521768  0.0000000000000012 20.4240737852088472   T   T   T
  1.3669039830006950  1.4493758552350018 19.3107709182549527   T   T   T
```

```
  7.2468792761750027  1.4493758552350009  9.2861208469999994   F   F   F
  7.2468792761750027  0.0000000000000005  8.0000000000000000   F   F   F
  9.4516698271584829  1.4493758552350009  9.2861208469999994   F   F   F
 10.8703189142625032  0.0000000000000006  9.2861208469999994   F   F   F
 10.8703189142625032  1.4493758552350011 12.5708101129999967   F   F   F
 10.8703189142625032  0.0000000000000007 11.2846892659999973   F   F   F
  7.2468792761750027  0.0000000000000006 10.5722416940000006   F   F   F
 12.2889680013665199  1.4493758552350009  9.2861208469999994   F   F   F
 13.0751094652459869  1.4493758552350011 12.5708101129999967   F   F   F
  7.2468792761750027  0.0000000000000008 12.5708101129999967   F   F   F
  6.8034601179481644  1.4493758552350011 15.8166410033310960   T   T   T
  7.1596545256280528  0.0000000000000009 14.6319810418051830   T   T   T
 10.8703189142625032  0.0000000000000008 13.8569309599999961   F   F   F
  8.6655283632790212  1.4493758552350011 12.5708101129999967   F   F   F
  9.5459526987656780  1.4493758552350011 15.8842188771808974   T   T   T
 10.7119282525872492  0.0000000000000009 15.9955212515408078   T   T   T
 10.5931833663772395  1.4493758552350018 19.3215228423101841   T   T   T
 10.8537402670201679  0.0000000000000011 17.8872637380443358   T   T   T
  7.1440782865877797  0.0000000000000010 17.1602862002452881   T   T   T
 12.2387297610948895  1.4493758552350011 15.8647946230608543   T   T   T
 13.3410249280685171  1.4493758552350018 19.4171598749634349   T   T   T
  7.2638149522763014  0.0000000000000011 19.0281012405203107   T   T   T
 10.8714865300333301  0.0000000000000012 20.4278026327692110   T   T   T
  8.6657937974422889  1.4493758552350018 19.2911565253177741   T   T   T

Metal reference: TiO2(110)/fcc(100)_5x1/Au E_tot= -50.01235623 eV
 D3-zero damping= -6.144536 eV, D3-BJ damping= -6.1920842 eV
Au
 1.0000000000000000
    14.4937585523500019    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8987517104700005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.4012876571641044
  15
Cartesian
  0.7248076056238033  0.0000000000000000  8.0938339186863146
  2.1722165629925114  1.4493758552350002 10.1858295308819287
  0.7201798647456781 -0.0000000000000002 12.2693961219849026
  3.6187436851640831 -0.0000000000000000  8.0898293880159500
  5.0679970431175860  1.4493758552350002 10.1841321919036094
  3.6205400412952184 -0.0000000000000000 12.2781406994410069
  6.5136841267961270 -0.0000000000000000  8.0898499644948885
  7.9682753269235880  1.4493758552350002 10.1807043658529164
  6.5184919805160986  0.0000000000000001 12.2704271220782157
  9.4168164121455824  0.0000000000000001  8.0887740264752725
 10.8627607085472047  1.4493758552350002 10.1885985359774143
  9.4157365267711839  0.0000000000000001 12.2796470651421394
 12.3107695697747150  0.0000000000000000  8.0909160706852727
 13.7603580485291559  1.4493758552350002 10.1801005685309374
 12.3168236891910379  0.0000000000000000 12.2788020256460513

Interface: TiO2(110)/fcc(100)_5x1/Ag E_tot= -466.66833654 eV
 D3-zero damping= -13.6601879 eV, D3-BJ damping= -16.6433744 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ag
 1.0000000000000000
    14.4026352597500011    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8805270519500006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.4839566596749165
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000007  1.4402635259750010  9.2861208469999976   F   F   F
  0.0000000000000005  0.0000000000000005  7.9999999999999982   F   F   F
```

2.1909288757131713	1.4402635259750010	9.2861208469999976	F	F	F
3.6006588149375012	0.0000000000000006	9.2861208469999976	F	F	F
3.6006588149375012	1.4402635259750012	12.5708101129999950	F	F	F
3.6006588149375012	0.0000000000000007	11.2846892659999956	F	F	F
0.0000000000000007	0.0000000000000006	10.5722416939999988	F	F	F
5.0103887541618315	1.4402635259750010	9.2861208469999976	F	F	F
5.7915876906506716	1.4402635259750012	12.5708101129999950	F	F	F
0.0000000000000008	0.0000000000000007	12.5708101129999950	F	F	F
14.1046673613440383	1.4402635259750012	15.8253862603280915	T	T	T
-0.0036385546156119	0.0000000000000069	14.6335057421014199	T	T	T
3.6006588149375012	0.0000000000000008	13.8569309599999944	F	F	F
1.4097299392243310	1.4402635259750012	12.5708101129999950	F	F	F
2.1873727791203570	1.4402635259750012	15.8260275795258600	T	T	T
3.3868949082138045	0.0000000000000016	15.8657873360232688	T	T	T
3.1417216937709638	1.4402635259750016	19.1916829478160373	T	T	T
3.3834684874763892	-0.0000000000000014	17.8521010541758969	T	T	T
14.3692149898056538	-0.0000000000000029	17.2211246539590874	T	T	T
4.8785695531218778	1.4402635259750012	15.9226938422744730	T	T	T
6.4501562182403873	1.4402635259750016	19.7058303077768642	T	T	T
-0.1204743344449409	0.0000000000000028	19.0704306553540555	T	T	T
3.6317363856493459	0.0000000000000032	20.3132168588509892	T	T	T
1.2526986927418846	1.4402635259750016	19.4447765398625165	T	T	T
7.2013176298750023	1.4402635259750010	9.2861208469999976	F	F	F
7.2013176298750023	0.0000000000000005	7.9999999999999982	F	F	F
9.3922465055881705	1.4402635259750010	9.2861208469999976	F	F	F
10.8019764448125031	0.0000000000000006	9.2861208469999976	F	F	F
10.8019764448125031	1.4402635259750012	12.5708101129999950	F	F	F
10.8019764448125031	0.0000000000000007	11.2846892659999956	F	F	F
7.2013176298750023	0.0000000000000006	10.5722416939999988	F	F	F
12.2117063840368321	1.4402635259750010	9.2861208469999976	F	F	F
12.9929053205256739	1.4402635259750012	12.5708101129999950	F	F	F
7.2013176298750023	0.0000000000000007	12.5708101129999950	F	F	F
6.7253152317134042	1.4402635259750012	15.8809914231055398	T	T	T
7.0954238422961113	0.0000000000000010	14.6899384043727324	T	T	T
10.8019764448125031	0.0000000000000008	13.8569309599999944	F	F	F
8.6110475690993322	1.4402635259750012	12.5708101129999950	F	F	F
9.5896097836677292	1.4402635259750012	15.9492633755267867	T	T	T
10.7649382870891515	0.0000000000000009	15.9038189733471391	T	T	T
10.8496190084409765	1.4402635259750016	19.2140102275694602	T	T	T
11.0218029458748283	0.0000000000000011	17.8816793441916460	T	T	T
7.0739174496527317	0.0000000000000009	17.2497333628859444	T	T	T
12.2648973460514767	1.4402635259750012	15.8320060623487961	T	T	T
13.0617598758336442	1.4402635259750016	19.3834645609282141	T	T	T
7.4936482178449637	0.0000000000000011	19.0851252955095667	T	T	T
10.9378047838238732	0.0000000000000012	20.4828619413284656	T	T	T
8.9037227356453368	1.4402635259750016	19.1732703037141015	T	T	T
0.9207053347966574	-0.0000000000000001	22.3018297548321982	T	T	T
2.2790576786817405	1.4402635259750003	24.4541181315913150	T	T	T
0.8046843153769206	0.0000000000000001	26.4179280005792307	T	T	T
3.7389253859210303	-0.0000000000000001	22.5081038742567543	T	T	T
5.1877906863396834	1.4402635259750003	24.4496848335645538	T	T	T
3.7304898382788871	-0.0000000000000000	26.4966897917373814	T	T	T
6.5460920980254222	0.0000000000000000	22.2945184222673660	T	T	T
8.0624347733069879	1.4402635259750003	24.2705979001862033	T	T	T
6.6703156584280157	-0.0000000000000000	26.4060796787255256	T	T	T
9.3668571410338028	0.0000000000000000	22.1956474369764010	T	T	T
10.9495893035427336	1.4402635259750003	24.1827075552818194	T	T	T
9.5305431286911304	-0.0000000000000000	26.2866915920225388	T	T	T
12.5277693060131377	-0.0000000000000000	22.1754974653788501	T	T	T
13.8068357553151007	1.4402635259750003	24.2812712379142006	T	T	T
12.3502821422392568	0.0000000000000000	26.3065924333564638	T	T	T

Oxide reference: TiO2(110)/fcc(100)_5x1/Ag E_tot= -422.60166923 eV

```
 D3-zero damping= -6.4820791 eV, D3-BJ damping= -9.0458522 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
    14.4026352597500011    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8805270519500006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.4556110558769895
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000007  1.4402635259750010  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  2.1909288757131713  1.4402635259750010  9.2861208469999994   F   F   F
  3.6006588149375012  0.0000000000000006  9.2861208469999994   F   F   F
  3.6006588149375012  1.4402635259750012 12.5708101129999967   F   F   F
  3.6006588149375012  0.0000000000000007 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416940000006   F   F   F
  5.0103887541618315  1.4402635259750010  9.2861208469999994   F   F   F
  5.7915876906506716  1.4402635259750012 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 14.0008467119016995  1.4402635259750012 15.8218684110772401   T   T   T
 -0.0569656669888348  0.0000000000000013 14.6330783130069797   T   T   T
  3.6006588149375012  0.0000000000000008 13.8569309599999961   F   F   F
  1.4097299392243310  1.4402635259750012 12.5708101129999967   F   F   F
  2.2680721035957037  1.4402635259750012 15.8794633043986053   T   T   T
  3.4469166829694271  0.0000000000000005 15.9982614447950553   T   T   T
  3.2844146198869519  1.4402635259750016 19.3336568620523437   T   T   T
  3.5445528608161205  0.0000000000000012 17.9018407691864248   T   T   T
 14.3210714245363864  0.0000000000000010 17.1767548862309205   T   T   T
  4.9634922026895998  1.4402635259750012 15.8846907124813175   T   T   T
  6.1130026484062343  1.4402635259750016 19.4558829570062777   T   T   T
 -0.0378894760700702  0.0000000000000011 19.0413313959809614   T   T   T
  3.5847861803103842  0.0000000000000012 20.4419765753102993   T   T   T
  1.3487108717406802  1.4402635259750016 19.3439716497988172   T   T   T
  7.2013176298750023  1.4402635259750010  9.2861208469999994   F   F   F
  7.2013176298750023  0.0000000000000005  8.0000000000000000   F   F   F
  9.3922465055881705  1.4402635259750010  9.2861208469999994   F   F   F
 10.8019764448125031  0.0000000000000006  9.2861208469999994   F   F   F
 10.8019764448125031  1.4402635259750012 12.5708101129999967   F   F   F
 10.8019764448125031  0.0000000000000007 11.2846892659999973   F   F   F
  7.2013176298750023  0.0000000000000006 10.5722416940000006   F   F   F
 12.2117063840368321  1.4402635259750010  9.2861208469999994   F   F   F
 12.9929053205256739  1.4402635259750012 12.5708101129999967   F   F   F
  7.2013176298750023  0.0000000000000007 12.5708101129999967   F   F   F
  6.7915582016660956  1.4402635259750012 15.8304097122019805   T   T   T
  7.1323691768832411  0.0000000000000009 14.6359471619404964   T   T   T
 10.8019764448125031  0.0000000000000008 13.8569309599999961   F   F   F
  8.6110475690993322  1.4402635259750012 12.5708101129999967   F   F   F
  9.4812105096100119  1.4402635259750012 15.8945185587928819   T   T   T
 10.6596371277671391  0.0000000000000009 16.0042887360828239   T   T   T
 10.5723039577159348  1.4402635259750016 19.3373392606725645   T   T   T
 10.8098500265761892  0.0000000000000010 17.8964058405708890   T   T   T
  7.1222016048093977  0.0000000000000010 17.1750600021023736   T   T   T
 12.1790419566755581  1.4402635259750012 15.8665156479979341   T   T   T
 13.2207018510111514  1.4402635259750016 19.4210558491370833   T   T   T
  7.2376362714269584  0.0000000000000011 19.0456976219772827   T   T   T
 10.8381514823360749  0.0000000000000012 20.4534977672223270   T   T   T
  8.6355676144101334  1.4402635259750016 19.3131449793047452   T   T   T

Metal reference: TiO2(110)/fcc(100)_5x1/Ag E_tot= -40.91565947 eV
 D3-zero damping= -4.5024555 eV, D3-BJ damping= -5.6711138 eV
Ag
 1.0000000000000000
```

```
    14.4026352597500011    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.8805270519500006    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.3020168036302238
  15
Cartesian
  0.8568557883334205 -0.0000000000000001  8.1007457052740239
  2.2989660043191882  1.4402635259750003 10.1506265966291789
  0.8567524213735754  0.0000000000000002 12.1984788244730407
  3.7356948202892921 -0.0000000000000000  8.0962355406352593
  5.1767384929559004  1.4402635259750003 10.1491323033746124
  3.7411145509172106 -0.0000000000000000 12.2022676939688477
  6.6153805413490190  0.0000000000000000  8.0963592589431919
  8.0592513864970847  1.4402635259750003 10.1467954498022532
  6.6215573950227373 -0.0000000000000000 12.1972543031595126
  9.4969562967879604  0.0000000000000000  8.0928828978310072
 10.9354855825888926  1.4402635259750003 10.1490041610925097
  9.4986423834857465 -0.0000000000000000 12.2016073182868858
 12.3771065861111484 -0.0000000000000000  8.0986214024663425
 13.8165830782204591  1.4402635259750003 10.1505162802902387
 12.3783471445757147  0.0000000000000000 12.2016205253874155

Interface: TiO2(110)/fcc(100)_5x1/Cu E_tot= -457.77180298 eV
 D3-zero damping= -14.0690462 eV, D3-BJ damping= -18.7949913 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Cu
 1.0000000000000000
    12.6188481836500017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.5237696367300004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.7626682023962488
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000006  1.2618848183650009  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  7.9999999999999991   F   F   F
  1.9195791856968392  1.2618848183650009  9.2861208469999994   F   F   F
  3.1547120459125013  0.0000000000000005  9.2861208469999994   F   F   F
  3.1547120459125013  1.2618848183650011 12.5708101129999967   F   F   F
  3.1547120459125013  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416939999988   F   F   F
  4.3898449061281637  1.2618848183650009  9.2861208469999994   F   F   F
  5.0742912316093394  1.2618848183650011 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000007 12.5708101129999967   F   F   F
 12.6641970581295293  1.2618848183650011 16.0663637286414414   T   T   T
  0.0525660809175840  0.0000000000000032 14.7089312892593060   T   T   T
  3.1547120459125013  0.0000000000000007 13.8569309599999961   F   F   F
  1.2351328602156628  1.2618848183650011 12.5708101129999967   F   F   F
  1.9577159355790843  1.2618848183650011 16.2337665755789757   T   T   T
  3.3130836685756613  0.0000000000000005 16.4643347682456067   T   T   T
  3.2030826948834354  1.2618848183650015 19.8812176711732747   T   T   T
  3.4140967086768756  0.0000000000000010 18.3782926884485498   T   T   T
 12.5718090875045601  0.0000000000000007 17.6004794820703623   T   T   T
  4.5310593801142920  1.2618848183650011 15.8286486980564849   T   T   T
  5.2625926125051876  1.2618848183650015 20.1234433003573443   T   T   T
 -0.1628790310944759  0.0000000000000007 19.4828057431513848   T   T   T
  3.2991318921107617  0.0000000000000010 21.3499247616212493   T   T   T
  1.2682982804234098  1.2618848183650015 19.8014143038811063   T   T   T
  6.3094240918250026  1.2618848183650009  9.2861208469999994   F   F   F
  6.3094240918250026  0.0000000000000004  7.9999999999999991   F   F   F
  8.2290032775218389  1.2618848183650009  9.2861208469999994   F   F   F
  9.4641361377375013  0.0000000000000005  9.2861208469999994   F   F   F
  9.4641361377375013  1.2618848183650011 12.5708101129999967   F   F   F
  9.4641361377375013  0.0000000000000006 11.2846892659999973   F   F   F
  6.3094240918250026  0.0000000000000006 10.5722416939999988   F   F   F
```

```
 10.6992689979531637  1.2618848183650009  9.2861208469999994   F   F   F
 11.3837153234343411  1.2618848183650011 12.5708101129999967   F   F   F
  6.3094240918250026  0.0000000000000007 12.5708101129999967   F   F   F
  6.4563652100365152  1.2618848183650011 16.0195890681066579   T   T   T
  6.6186751247367006  0.0000000000000008 14.6796270699535167   T   T   T
  9.4641361377375013  0.0000000000000007 13.8569309599999961   F   F   F
  7.5445569520406641  1.2618848183650011 12.5708101129999967   F   F   F
  8.2723596960560037  1.2618848183650011 16.7107767581521642   T   T   T
  9.6512338540969420  0.0000000000000008 16.9447285243808459   T   T   T
  9.6130297855380515  1.2618848183650015 20.2942160242887830   T   T   T
 10.1572915398231505  0.0000000000000008 18.7857033128201607   T   T   T
  6.0915023075738111  0.0000000000000009 17.5126677949024341   T   T   T
 10.7160107879148558  1.2618848183650011 16.0891211505576628   T   T   T
 11.5226478817560274  1.2618848183650015 20.7140856321771096   T   T   T
  6.4016704586423634  0.0000000000000010 19.3068917953724437   T   T   T
  8.9477463950865523  0.0000000000000010 21.6113597486561275   T   T   T
  7.8011789479499027  1.2618848183650015 19.5164982135734704   T   T   T
 -0.2652448711258336 -0.0000000000000001 23.0375237320004160   T   T   T
  1.0406431974585286  1.2618848183650002 24.7702921247382974   T   T   T
 -0.1628740906474709  0.0000000000000001 26.6505480847002509   T   T   T
  2.1802342028887436  0.0000000000000001 22.9385012016191254   T   T   T
  3.5571705371433353  1.2618848183650002 24.6689929474468315   T   T   T
  2.3397693228123582  0.0000000000000000 26.5109251946655924   T   T   T
  4.8279660323835003  0.0000000000000000 22.7919221583026399   T   T   T
  6.0600938953006107  1.2618848183650002 24.6353765987043474   T   T   T
  4.8085303711795317 -0.0000000000000000 26.4565809381133654   T   T   T
  7.3701888580622752 -0.0000000000000000 22.9304706833442964   T   T   T
  8.5650885558602834  1.2618848183650002 24.9074284091862168   T   T   T
  7.2647925668715558 -0.0000000000000001 26.5822002082424120   T   T   T
  9.9414396524012201  0.0000000000000000 23.2613369873393516   T   T   T
 11.1506528797931246  1.2618848183650002 24.9566787383261151   T   T   T
  9.8356175316570429  0.0000000000000000 26.6887244973686784   T   T   T

Oxide reference: TiO2(110)/fcc(100)_5x1/Cu E_tot= -399.84265741 eV
 D3-zero damping= -7.8189333 eV, D3-BJ damping= -11.2850261 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
    12.6188481836500017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.5237696367300004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   29.4861880028888770
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000006  1.2618848183650009  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  8.0000000000000000   F   F   F
  1.9195791856968392  1.2618848183650009  9.2861208469999994   F   F   F
  3.1547120459125013  0.0000000000000005  9.2861208469999994   F   F   F
  3.1547120459125013  1.2618848183650011 12.5708101129999967   F   F   F
  3.1547120459125013  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000006  0.0000000000000006 10.5722416940000006   F   F   F
  4.3898449061281637  1.2618848183650009  9.2861208469999994   F   F   F
  5.0742912316093394  1.2618848183650011 12.5708101129999967   F   F   F
  0.0000000000000007  0.0000000000000007 12.5708101129999967   F   F   F
 12.6762305841330924  1.2618848183650011 16.0611948621629352   T   T   T
  0.1644912761513388  0.0000000000000002 14.7131302587081425   T   T   T
  3.1547120459125013  0.0000000000000007 13.8569309599999961   F   F   F
  1.2351328602156628  1.2618848183650011 12.5708101129999967   F   F   F
  1.9354637399285244  1.2618848183650011 16.5406418169327161   T   T   T
  3.2988842635499949  0.0000000000000002 16.8056789756195251   T   T   T
  3.3507996221785818  1.2618848183650015 20.2272548225540305   T   T   T
  3.5954583502918136  0.0000000000000009 18.6390466257487972   T   T   T
 12.4665528583892407  0.0000000000000010 17.5847739485953376   T   T   T
```

```
  4.4251241528777596  1.2618848183650011 16.0082044008173163   T   T   T
  5.3195405281153256  1.2618848183650015 20.3675847369561289   T   T   T
  0.0645731130123275  0.0000000000000011 19.4197200839288620   T   T   T
  3.0845359408429136  0.0000000000000010 21.4879118337769803   T   T   T
  1.4300250259949403  1.2618848183650015 19.6617221780784988   T   T   T
  6.3094240918250026  1.2618848183650009  9.2861208469999994   F   F   F
  6.3094240918250026  0.0000000000000004  8.0000000000000000   F   F   F
  8.2290032775218389  1.2618848183650009  9.2861208469999994   F   F   F
  9.4641361377375013  0.0000000000000005  9.2861208469999994   F   F   F
  9.4641361377375013  1.2618848183650011 12.5708101129999967   F   F   F
  9.4641361377375013  0.0000000000000006 11.2846892659999973   F   F   F
  6.3094240918250026  0.0000000000000006 10.5722416940000006   F   F   F
 10.6992689979531637  1.2618848183650009  9.2861208469999994   F   F   F
 11.3837153234343411  1.2618848183650011 12.5708101129999967   F   F   F
  6.3094240918250026  0.0000000000000007 12.5708101129999967   F   F   F
  6.3631822039380435  1.2618848183650011 16.0602647810462784   T   T   T
  6.4640230177853235  0.0000000000000008 14.7117648543741701   T   T   T
  9.4641361377375013  0.0000000000000007 13.8569309599999961   F   F   F
  7.5445569520406641  1.2618848183650011 12.5708101129999967   F   F   F
  8.2444033059650703  1.2618848183650011 16.5244006055111576   T   T   T
  9.6078399717292715  0.0000000000000008 16.7907633432894663   T   T   T
  9.6563293805585264  1.2618848183650015 20.2125013907041229   T   T   T
  9.8943706840428245  0.0000000000000009 18.6248594713273974   T   T   T
  6.1583296048211880  0.0000000000000009 17.5838691267816039   T   T   T
 10.7398347905727487  1.2618848183650011 16.0012153450836934   T   T   T
 11.6260093585445308  1.2618848183650015 20.3538476052424855   T   T   T
  6.3676727959822923  0.0000000000000010 19.4207848674890080   T   T   T
  9.3937818862422287  0.0000000000000010 21.4740388565803748   T   T   T
  7.7336807535944212  1.2618848183650015 19.6555959081667098   T   T   T

Metal reference: TiO2(110)/fcc(100)_5x1/Cu E_tot= -54.41677682 eV
 D3-zero damping= -4.2998545 eV, D3-BJ damping= -5.4413004 eV
Cu
 1.0000000000000000
    12.6188481836500017    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.5237696367300004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.8329203848584790
  15
Cartesian
 -0.1176647919915383 -0.0000000000000001  8.1787734201490636
  1.1432680347152893  1.2618848183650002  9.9636915776723587
 -0.1169354859884234  0.0000000000000000 11.7492786191192913
  2.4058498002043072  0.0000000000000001  8.1799252428740203
  3.6673159246225908  1.2618848183650002  9.9632412468498277
  2.4054133571721552  0.0000000000000000 11.7474503807901076
  4.9295371232990064  0.0000000000000000  8.1802340749530167
  6.1920387830900179  1.2618848183650002  9.9619412565525174
  4.9305581649025871 -0.0000000000000001 11.7457331609376823
  7.4562583847474375 -0.0000000000000000  8.1797623319517960
  8.7162075965270116  1.2618848183650002  9.9646026026543009
  7.4528224324696302 -0.0000000000000001 11.7475532774363316
  9.9771956487325717  0.0000000000000000  8.1810991913510609
 11.2397673293008236  1.2618848183650002  9.9644983331595594
  9.9766902756774805 -0.0000000000000000 11.7484371940716663

Interface: TiO2(110)/fcc(100)_5x1/Pt E_tot= -515.70807338 eV
 D3-zero damping= -16.7125006 eV, D3-BJ damping= -19.2633606 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Pt
 1.0000000000000000
    13.8522668271000011    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7704533654200003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.3490071247424780
```

```
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000007  1.3852266827100008  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  7.9999999999999991   F   F   F
  2.1072068297384532  1.3852266827100008  9.2861208469999994   F   F   F
  3.4630667067750012  0.0000000000000005  9.2861208469999994   F   F   F
  3.4630667067750012  1.3852266827100010 12.5708101129999967   F   F   F
  3.4630667067750012  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416939999988   F   F   F
  4.8189265838115496  1.3852266827100008  9.2861208469999994   F   F   F
  5.5702735365134535  1.3852266827100010 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 13.6456927393962246  1.3852266827100010 15.9732681672122361   T   T   T
 -0.0267823062392278  0.0000000000000009 14.6577493125014247   T   T   T
  3.4630667067750012  0.0000000000000008 13.8569309599999961   F   F   F
  1.3558598770365489  1.3852266827100010 12.5708101129999967   F   F   F
  2.1245870306115875  1.3852266827100010 15.9112884732105222   T   T   T
  3.3921894795672016  0.0000000000000005 15.9197319325608930   T   T   T
  3.2567647080451971  1.3852266827100015 19.2371574364684719   T   T   T
  3.4850420037326519  0.0000000000000012 17.9074994777840182   T   T   T
 13.8020474080757722  0.0000000000000009 17.3063291661518619   T   T   T
  4.8330436225855200  1.3852266827100010 15.8935607543117676   T   T   T
  5.6212389145250414  1.3852266827100015 19.4458535119415323   T   T   T
 -0.0942401212753931  0.0000000000000011 19.4098591108778606   T   T   T
  3.4753235519075028  0.0000000000000012 20.5230077664863444   T   T   T
  1.3182159097826971  1.3852266827100015 19.3233263942644200   T   T   T
  6.9261334135500023  1.3852266827100008  9.2861208469999994   F   F   F
  6.9261334135500023  0.0000000000000005  7.9999999999999991   F   F   F
  9.0333402432884533  1.3852266827100008  9.2861208469999994   F   F   F
 10.3892001203250022  0.0000000000000005  9.2861208469999994   F   F   F
 10.3892001203250022  1.3852266827100010 12.5708101129999967   F   F   F
 10.3892001203250022  0.0000000000000006 11.2846892659999973   F   F   F
  6.9261334135500023  0.0000000000000006 10.5722416939999988   F   F   F
 11.7450599973615493  1.3852266827100008  9.2861208469999994   F   F   F
 12.4964069500634558  1.3852266827100010 12.5708101129999967   F   F   F
  6.9261334135500023  0.0000000000000007 12.5708101129999967   F   F   F
  6.7533061074381360  1.3852266827100010 15.9087689593857906   T   T   T
  6.9204883095501781  0.0000000000000009 14.6417066144398014   T   T   T
 10.3892001203250022  0.0000000000000008 13.8569309599999961   F   F   F
  8.2819932905865503  1.3852266827100010 12.5708101129999967   F   F   F
  8.9909997832965853  1.3852266827100010 15.8973313177996562   T   T   T
 10.2874942076353477  0.0000000000000009 15.9236126521928636   T   T   T
 10.2608618065148764  1.3852266827100015 19.2658440985255410   T   T   T
 10.3154352759664913  0.0000000000000010 17.9262711220746240   T   T   T
  6.9005942102869335  0.0000000000000010 17.2955115669000001   T   T   T
 11.6850972929594388  1.3852266827100010 15.9282756658798128   T   T   T
 12.4518240094846675  1.3852266827100015 19.3660384974519353   T   T   T
  6.8810768543795984  0.0000000000000011 19.2002319418533958   T   T   T
 10.3517871033805697  0.0000000000000012 20.5826322373401105   T   T   T
  8.2579438290720368  1.3852266827100015 19.4179549053632847   T   T   T
  0.0852234178537710  0.0000000000000000 22.0687919209009067   T   T   T
  1.4255566876945915  1.3852266827100002 24.3305174523535719   T   T   T
  0.0576431379717571  0.0000000000000000 26.2630802084963086   T   T   T
  2.7195822797147096  0.0000000000000000 22.4169591080193342   T   T   T
  4.1993895408396691  1.3852266827100002 24.3688533472943831   T   T   T
  2.8414023842119405  0.0000000000000000 26.3244345279541321   T   T   T
  5.6240259712005018 -0.0000000000000000 22.4322174826076832   T   T   T
  6.9787907129202553  1.3852266827100002 24.3987019325835313   T   T   T
  5.6062365973415220  0.0000000000000000 26.3280189142261065   T   T   T
  8.2746364279863052  0.0000000000000000 22.4012358268068503   T   T   T
  9.7734385943188506  1.3852266827100002 24.2817878861233858   T   T   T
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  8.4052670612828475  0.0000000000000000 26.2817357875308986   T   T   T
 11.3123928739603556 -0.0000000000000000 22.3829056342815456   T   T   T
 12.5797179677333464  1.3852266827100002 24.3000648793788834   T   T   T
 11.1355650633252434  0.0000000000000000 26.2543444922383031   T   T   T

Oxide reference: TiO2(110)/fcc(100)_5x1/Pt E_tot= -422.65187718 eV
 D3-zero damping= -6.902324 eV, D3-BJ damping= -9.7399805 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
    13.8522668271000011    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7704533654200003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6264844381430130
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000007  1.3852266827100008  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  2.1072068297384532  1.3852266827100008  9.2861208469999994   F   F   F
  3.4630667067750012  0.0000000000000005  9.2861208469999994   F   F   F
  3.4630667067750012  1.3852266827100010 12.5708101129999967   F   F   F
  3.4630667067750012  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416940000006   F   F   F
  4.8189265838115496  1.3852266827100008  9.2861208469999994   F   F   F
  5.5702735365134535  1.3852266827100010 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 13.6075666734282681  1.3852266827100010 15.8839792947519989   T   T   T
 -0.0130345582150335  0.0000000000000011 14.6422867992026671   T   T   T
  3.4630667067750012  0.0000000000000008 13.8569309599999961   F   F   F
  1.3558598770365489  1.3852266827100010 12.5708101129999967   F   F   F
  2.0855994919273591  1.3852266827100010 15.9281668067525572   T   T   T
  3.3451110590062081  0.0000000000000005 16.0606683200123790   T   T   T
  3.3181259787523052  1.3852266827100015 19.4460527725055954   T   T   T
  3.4278695134167165  0.0000000000000011 17.9747372858438865   T   T   T
 13.8304463363573227  0.0000000000000009 17.2671597157305285   T   T   T
  4.8020975571264648  1.3852266827100010 15.9267069660077905   T   T   T
  5.6338059308591184  1.3852266827100015 19.4734437167107828   T   T   T
 -0.0472124477707635  0.0000000000000011 19.1362307678362882   T   T   T
  3.4745943327315469  0.0000000000000012 20.6270857893060793   T   T   T
  1.2921264205497884  1.3852266827100015 19.4833799246985997   T   T   T
  6.9261334135500023  1.3852266827100008  9.2861208469999994   F   F   F
  6.9261334135500023  0.0000000000000005  8.0000000000000000   F   F   F
  9.0333402432884533  1.3852266827100008  9.2861208469999994   F   F   F
 10.3892001203250022  0.0000000000000005  9.2861208469999994   F   F   F
 10.3892001203250022  1.3852266827100010 12.5708101129999967   F   F   F
 10.3892001203250022  0.0000000000000006 11.2846892659999973   F   F   F
  6.9261334135500023  0.0000000000000006 10.5722416940000006   F   F   F
 11.7450599973615493  1.3852266827100008  9.2861208469999994   F   F   F
 12.4964069500634558  1.3852266827100010 12.5708101129999967   F   F   F
  6.9261334135500023  0.0000000000000007 12.5708101129999967   F   F   F
  6.6813492874658138  1.3852266827100010 15.8838354574311467   T   T   T
  6.9126161147031873  0.0000000000000009 14.6420711926170597   T   T   T
 10.3892001203250022  0.0000000000000008 13.8569309599999961   F   F   F
  8.2819932905865503  1.3852266827100010 12.5708101129999967   F   F   F
  9.0115431825043579  1.3852266827100010 15.9271294819897289   T   T   T
 10.2711025041698534  0.0000000000000009 16.0597568301115636   T   T   T
 10.2443922600130009  1.3852266827100015 19.4448052262909208   T   T   T
 10.3540941390013970  0.0000000000000010 17.9735901267833320   T   T   T
  6.9045893166752146  0.0000000000000010 17.2668368796485510   T   T   T
 11.7282799346656201  1.3852266827100010 15.9259113511436183   T   T   T
 12.5599455152561692  1.3852266827100015 19.4736481930686658   T   T   T
  6.8790191257115874  0.0000000000000011 19.1358683885508469   T   T   T
 10.4002748594025114  0.0000000000000012 20.6257904669757259   T   T   T
```

```
  8.2183413143670059  1.3852266827100015 19.4824787377313662   T   T   T

Metal reference: TiO2(110)/fcc(100)_5x1/Pt E_tot= -89.60780279 eV
 D3-zero damping= -6.8694538 eV, D3-BJ damping= -7.1994921 eV
Pt
 1.0000000000000000
    13.8522668271000011    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7704533654200003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.2990840521110520
  15
Cartesian
  0.0434888251991575  0.0000000000000001  8.3243918062689612
  1.4311876491695583  1.3852266827100002 10.2740364357757237
  0.0472103452578985  0.0000000000000000 12.2218216568308495
  2.8160689347059571  0.0000000000000000  8.3282467028961307
  4.2034574133471194  1.3852266827100002 10.2774657076103644
  2.8165088406490848  0.0000000000000000 12.2227596126624807
  5.5845349042375201 -0.0000000000000000  8.3271042829167694
  6.9734537530767193  1.3852266827100002 10.2761388210576676
  5.5891181576027877  0.0000000000000000 12.2249646241632028
  8.3531328157724953  0.0000000000000000  8.3248435975899913
  9.7421248567870720  1.3852266827100002 10.2740458592624488
  8.3612808196147981  0.0000000000000000 12.2237768414106949
 11.1236820010200361 -0.0000000000000000  8.3253383727365744
 12.5128388438018572  1.3852266827100002 10.2733204093398776
 11.1303814319448815  0.0000000000000000 12.2210444539623708

Interface: TiO2(110)/fcc(100)_5x1/Pd E_tot= -501.9880997 eV
 D3-zero damping= -15.1014735 eV, D3-BJ damping= -18.3556889 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Pd
 1.0000000000000000
    13.7399061595000003    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7479812319000003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.3091026375017734
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000007  1.3739906159500008  9.2861208469999976   F   F   F
  0.0000000000000005  0.0000000000000005  7.9999999999999982   F   F   F
  2.0901145249831412  1.3739906159500008  9.2861208469999976   F   F   F
  3.4349765398750010  0.0000000000000005  9.2861208469999976   F   F   F
  3.4349765398750010  1.3739906159500010 12.5708101129999950   F   F   F
  3.4349765398750010  0.0000000000000006 11.2846892659999956   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416939999988   F   F   F
  4.7798385547668616  1.3739906159500008  9.2861208469999976   F   F   F
  5.5250910648581408  1.3739906159500010 12.5708101129999950   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999950   F   F   F
 13.6210813294143058  1.3739906159500010 15.9629645943553182   T   T   T
 -0.0073976811407254  0.0000000000000015 14.6711594270014132   T   T   T
  3.4349765398750010  0.0000000000000008 13.8569309599999944   F   F   F
  1.3448620148918609  1.3739906159500010 12.5708101129999950   F   F   F
  2.0642863728968681  1.3739906159500010 15.9331717102696100   T   T   T
  3.3772112688976930  0.0000000000000006 15.9585221995605071   T   T   T
  3.4311272878913539  1.3739906159500015 19.3220370602084621   T   T   T
  3.4304720800418145  0.0000000000000011 17.9454722164405673   T   T   T
 13.7289667227212551  0.0000000000000009 17.3654566686114578   T   T   T
  4.7884892040919267  1.3739906159500010 15.9135129937937627   T   T   T
  5.5455635925654168  1.3739906159500015 19.3958362792239818   T   T   T
  0.0014454981885913  0.0000000000000011 19.3040732727633859   T   T   T
  3.6078024463203109  0.0000000000000012 20.6222602019139813   T   T   T
  1.3511896052406209  1.3739906159500015 19.4949362812550078   T   T   T
  6.8699530797500019  1.3739906159500008  9.2861208469999976   F   F   F
```

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  6.8699530797500019  0.0000000000000005  7.9999999999999982   F   F   F
  8.9600676047331405  1.3739906159500008  9.2861208469999976   F   F   F
 10.3049296196250015  0.0000000000000005  9.2861208469999976   F   F   F
 10.3049296196250015  1.3739906159500010 12.5708101129999950   F   F   F
 10.3049296196250015  0.0000000000000006 11.2846892659999956   F   F   F
  6.8699530797500019  0.0000000000000006 10.5722416939999988   F   F   F
 11.6497916345168608  1.3739906159500008  9.2861208469999976   F   F   F
 12.3950441446081427  1.3739906159500010 12.5708101129999950   F   F   F
  6.8699530797500019  0.0000000000000007 12.5708101129999950   F   F   F
  6.7466288564442527  1.3739906159500010 15.9016928770912802   T   T   T
  6.8719146595663254  0.0000000000000009 14.6250986382528438   T   T   T
 10.3049296196250015  0.0000000000000008 13.8569309599999944   F   F   F
  8.2148150946418621  1.3739906159500010 12.5708101129999950   F   F   F
  8.9334108665223209  1.3739906159500010 15.9219817868261799   T   T   T
 10.2477126745017824  0.0000000000000009 15.9650568300131930   T   T   T
 10.3203094194308811  1.3739906159500015 19.3339601002581034   T   T   T
 10.2946612002995259  0.0000000000000010 17.9597409563249570   T   T   T
  6.8659050778586668  0.0000000000000010 17.2797451217177169   T   T   T
 11.6531535358108105  1.3739906159500010 15.9409397652066307   T   T   T
 12.3850546442578597  1.3739906159500015 19.5034796279474563   T   T   T
  6.8716028426618259  0.0000000000000011 19.1783870587004088   T   T   T
 10.1192245561314298  0.0000000000000011 20.6398343505007063   T   T   T
  8.1887932735494093  1.3739906159500015 19.3976337778478012   T   T   T
  0.0419815753925459  0.0000000000000000 22.2534480975552640   T   T   T
  1.3852519521403130  1.3739906159500002 24.3560964399599200   T   T   T
  0.0364806327070248  0.0000000000000000 26.3148152240466118   T   T   T
  2.6506057969022363  0.0000000000000000 22.4357680982798549   T   T   T
  4.1974140497751717  1.3739906159500002 24.2466589383400901   T   T   T
  2.8382719884673202  0.0000000000000000 26.2403370953204487   T   T   T
  5.5323806519001506  0.0000000000000000 22.1582729190379446   T   T   T
  6.9082255558194969  1.3739906159500002 24.1295055958003708   T   T   T
  5.5792927862580504 -0.0000000000000000 26.1673641427900954   T   T   T
  8.2655939294315406  0.0000000000000000 22.1544836308840196   T   T   T
  9.6265580098256898  1.3739906159500002 24.2281758988045226   T   T   T
  8.2499918906898646 -0.0000000000000000 26.1524223455872615   T   T   T
 11.1729215842860974  0.0000000000000000 22.4142444700318322   T   T   T
 12.4353585256349657  1.3739906159500002 24.3423856297060404   T   T   T
 10.9850398426188285  0.0000000000000000 26.2271390512673825   T   T   T

Oxide reference: TiO2(110)/fcc(100)_5x1/Pd E_tot= -422.11351834 eV
 D3-zero damping= -6.9864711 eV, D3-BJ damping= -9.8852473 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
    13.7399061595000003    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7479812319000003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.6711539050071629
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000007  1.3739906159500008  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000005  8.0000000000000000   F   F   F
  2.0901145249831412  1.3739906159500008  9.2861208469999994   F   F   F
  3.4349765398750010  0.0000000000000005  9.2861208469999994   F   F   F
  3.4349765398750010  1.3739906159500010 12.5708101129999967   F   F   F
  3.4349765398750010  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416940000006   F   F   F
  4.7798385547668616  1.3739906159500008  9.2861208469999994   F   F   F
  5.5250910648581408  1.3739906159500010 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 13.5450136100680094  1.3739906159500010 15.8987008972883981   T   T   T
 -0.0003828134551263  0.0000000000000015 14.6453335997997769   T   T   T
  3.4349765398750010  0.0000000000000008 13.8569309599999961   F   F   F
```

```
  1.3448620148918609  1.3739906159500010 12.5708101129999967   F   F   F
  2.0602281625387762  1.3739906159500010 15.9449323166641665   T   T   T
  3.3374415393724752  0.0000000000000006 16.0809241166173500   T   T   T
  3.5226969612588945  1.3739906159500015 19.4758591522076259   T   T   T
  3.4271205578958512  0.0000000000000012 17.9956157566526613   T   T   T
 13.7386308695912103  0.0000000000000010 17.2923301408319254   T   T   T
  4.7790478852655731  1.3739906159500010 15.9369300909611464   T   T   T
  5.5724633100306464  1.3739906159500015 19.5104419097637987   T   T   T
  0.0302817720918350  0.0000000000000011 19.1596359232213977   T   T   T
  3.4179898032745877  0.0000000000000012 20.6715393193439567   T   T   T
  1.2907528898263281  1.3739906159500015 19.5057648242194723   T   T   T
  6.8699530797500019  1.3739906159500008  9.2861208469999994   F   F   F
  6.8699530797500019  0.0000000000000005  8.0000000000000000   F   F   F
  8.9600676047331405  1.3739906159500008  9.2861208469999994   F   F   F
 10.3049296196250015  0.0000000000000005  9.2861208469999994   F   F   F
 10.3049296196250015  1.3739906159500010 12.5708101129999967   F   F   F
 10.3049296196250015  0.0000000000000006 11.2846892659999973   F   F   F
  6.8699530797500019  0.0000000000000006 10.5722416940000006   F   F   F
 11.6497916345168608  1.3739906159500008  9.2861208469999994   F   F   F
 12.3950441446081427  1.3739906159500010 12.5708101129999967   F   F   F
  6.8699530797500019  0.0000000000000007 12.5708101129999967   F   F   F
  6.6752812409127467  1.3739906159500010 15.8983234308372765   T   T   T
  6.8694673277262028  0.0000000000000009 14.6448491180595379   T   T   T
 10.3049296196250015  0.0000000000000008 13.8569309599999961   F   F   F
  8.2148150946418621  1.3739906159500010 12.5708101129999967   F   F   F
  8.9303230712976021  1.3739906159500010 15.9447753910135486   T   T   T
 10.2076174690668608  0.0000000000000009 16.0801330931844717   T   T   T
 10.3926652189658668  1.3739906159500015 19.4754014929140098   T   T   T
 10.2979640148822540  0.0000000000000010 17.9950044076071087   T   T   T
  6.8691182059070348  0.0000000000000010 17.2919852719645526   T   T   T
 11.6486783543173065  1.3739906159500010 15.9364355165363722   T   T   T
 12.4428018072191158  1.3739906159500015 19.5113742982763014   T   T   T
  6.9001017853067568  0.0000000000000011 19.1590934788471543   T   T   T
 10.2874573851755944  0.0000000000000011 20.6710379894688430   T   T   T
  8.1607135788879610  1.3739906159500015 19.5045464706986102   T   T   T

Metal reference: TiO2(110)/fcc(100)_5x1/Pd E_tot= -76.18592172 eV
 D3-zero damping= -5.089321 eV, D3-BJ damping= -6.218495 eV
Pd
 1.0000000000000000
    13.7399061595000003    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7479812319000003    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.1437878729837294
  15
Cartesian
  0.0398461659719755  0.0000000000000001  8.1333170608707963
  1.4134067151480110  1.3739906159500002 10.0969044247550173
  0.0388085843698665  0.0000000000000000 12.0555402685936155
  2.7863160990856342  0.0000000000000000  8.1371399008618237
  4.1608547937454183  1.3739906159500002 10.0977442296972537
  2.7884895856365377  0.0000000000000000 12.0564569728561786
  5.5343661054058026  0.0000000000000000  8.1387759248223208
  6.9117888677809116  1.3739906159500002 10.0946312958124427
  5.5387537456539313 -0.0000000000000000 12.0532954262537810
  8.2834791860478223  0.0000000000000000  8.1352171610000710
  9.6613041816888501  1.3739906159500002 10.0926912493616001
  8.2848164075378499 -0.0000000000000000 12.0513857237796849
 11.0331786155459248  0.0000000000000000  8.1314498335734235
 12.4066632084276751  1.3739906159500002 10.0942962335599429
 11.0315689765334053  0.0000000000000000 12.0530521129707218

Interface: TiO2(110)/fcc(100)_5x1/Ir E_tot= -550.7779593 eV
 D3-zero damping= -15.9673539 eV, D3-BJ damping= -19.1060526 eV
```

```
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ir
 1.0000000000000000
    13.5753160727500024    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7150632145500007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.2500268627094400
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000007  1.3575316072750010  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  8.0000000000000000   F   F   F
  2.0650770809867316  1.3575316072750010  9.2861208469999994   F   F   F
  3.3938290181875015  0.0000000000000005  9.2861208469999994   F   F   F
  3.3938290181875015  1.3575316072750012 12.5708101129999967   F   F   F
  3.3938290181875015  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416940000006   F   F   F
  4.7225809553882723  1.3575316072750010  9.2861208469999994   F   F   F
  5.4589060991742322  1.3575316072750012 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 13.5876837482897770  1.3575316072750012 15.9444840345114152   T   T   T
 -0.0195812477843043  0.0000000000000026 14.6415569702164312   T   T   T
  3.3938290181875015  0.0000000000000008 13.8569309599999961   F   F   F
  1.3287519372007710  1.3575316072750012 12.5708101129999967   F   F   F
  2.0286049899684175  1.3575316072750012 15.9082044291076112   T   T   T
  3.3971873199473421  0.0000000000000005 15.9124492917832203   T   T   T
  3.3923430186796639  1.3575316072750017 19.2615056295433895   T   T   T
  3.3949641823442231  0.0000000000000013 17.8999711861682371   T   T   T
 13.5773728369651607  0.0000000000000011 17.3582255730679549   T   T   T
  4.7633244292044603  1.3575316072750012 15.9075672668312063   T   T   T
  5.4606137086052664  1.3575316072750017 19.4680576815446678   T   T   T
 -0.0104506013793777  0.0000000000000009 19.2630462351416014   T   T   T
  3.3935735073583868  0.0000000000000011 20.5875996481204488   T   T   T
  1.3265742929348872  1.3575316072750017 19.4678287287047169   T   T   T
  6.7876580363750030  1.3575316072750010  9.2861208469999994   F   F   F
  6.7876580363750030  0.0000000000000004  8.0000000000000000   F   F   F
  8.8527351173617319  1.3575316072750010  9.2861208469999994   F   F   F
 10.1814870545625027  0.0000000000000005  9.2861208469999994   F   F   F
 10.1814870545625027  1.3575316072750012 12.5708101129999967   F   F   F
 10.1814870545625027  0.0000000000000006 11.2846892659999973   F   F   F
  6.7876580363750030  0.0000000000000006 10.5722416940000006   F   F   F
 11.5102389917632735  1.3575316072750010  9.2861208469999994   F   F   F
 12.2465641355492352  1.3575316072750012 12.5708101129999967   F   F   F
  6.7876580363750030  0.0000000000000007 12.5708101129999967   F   F   F
  6.7843498887144502  1.3575316072750012 15.9439653021918737   T   T   T
  6.8098362811203907  0.0000000000000008 14.6410502884342186   T   T   T
 10.1814870545625027  0.0000000000000008 13.8569309599999961   F   F   F
  8.1164099735757738  1.3575316072750012 12.5708101129999967   F   F   F
  8.8271304906805774  1.3575316072750012 15.9635845452371008   T   T   T
 10.1838181734483761  0.0000000000000009 15.9624192663101923   T   T   T
 10.1804619089127861  1.3575316072750017 19.3751652845000599   T   T   T
 10.1813844035439001  0.0000000000000009 18.0125555916326974   T   T   T
  6.7878191591982873  0.0000000000000010 17.3577336921775434   T   T   T
 11.5387884453202822  1.3575316072750012 15.9636459827444046   T   T   T
 12.2158201874045691  1.3575316072750017 19.4968345529359048   T   T   T
  6.7968379348633965  0.0000000000000011 19.2619767610648864   T   T   T
 10.1791229874107181  0.0000000000000011 20.8376524030035881   T   T   T
  8.1458307764200732  1.3575316072750017 19.4967925060494203   T   T   T
  0.6648330643306138  0.0000000000000001 22.5066351680718668   T   T   T
  2.0292167942296526  1.3575316452422317 24.3949690363183365   T   T   T
  0.6540447182818118  0.0000000000000000 26.2382331133850641   T   T   T
  3.3889941119216109  0.0000000000000001 22.5644703054259566   T   T   T
  4.7489593427351098  1.3575316072750003 24.3950583462874775   T   T   T
  3.3893615439001672 -0.0000000000000001 26.2526669327650382   T   T   T
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  6.1139965601798325  0.0000000000000000 22.5071362588602106   T   T   T
  7.4639944088095014  1.3575316072750003 24.3525341181851722   T   T   T
  6.1246061522862147 -0.0000000000000000 26.2379296690042167   T   T   T
  8.7629125129827159 -0.0000000000000000 22.4724720038765788   T   T   T
 10.1769462096800662  1.3575316072750003 24.3375390268443432   T   T   T
  8.8334597367153158  0.0000000000000000 26.1892089259470602   T   T   T
 11.5915297869905878 -0.0000000000000000 22.4726771890236172   T   T   T
 12.8900073641201534  1.3575316072750003 24.3524340215000947   T   T   T
 11.5201986054334906 -0.0000000000000000 26.1892497972005138   T   T   T

Oxide reference: TiO2(110)/fcc(100)_5x1/Ir E_tot= -420.84806891 eV
 D3-zero damping= -7.1075453 eV, D3-BJ damping= -10.1012089 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
    13.575316072750002 4    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7150632145500007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.7334962738331789
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000007  1.3575316072750010  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  8.0000000000000000   F   F   F
  2.0650770809867316  1.3575316072750010  9.2861208469999994   F   F   F
  3.3938290181875015  0.0000000000000005  9.2861208469999994   F   F   F
  3.3938290181875015  1.3575316072750012 12.5708101129999967   F   F   F
  3.3938290181875015  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416940000006   F   F   F
  4.7225809553882723  1.3575316072750010  9.2861208469999994   F   F   F
  5.4589060991742322  1.3575316072750012 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 13.4678293914328400  1.3575316072750012 15.9171546670063950   T   T   T
 -0.0015838519952451  0.0000000000000012 14.6471708858757559   T   T   T
  3.3938290181875015  0.0000000000000008 13.8569309599999961   F   F   F
  1.3287519372007710  1.3575316072750012 12.5708101129999967   F   F   F
  2.0182014771419872  1.3575316072750012 15.9584889441562883   T   T   T
  3.3335048904698779  0.0000000000000005 16.1115755014011057   T   T   T
  3.3920720197360281  1.3575316072750017 19.5219239494574559   T   T   T
  3.3734092189557661  0.0000000000000010 18.0272292036713111   T   T   T
 13.5736926731110401  0.0000000000000010 17.3286205926368417   T   T   T
  4.7364996637245387  1.3575316072750012 15.9601162111694777   T   T   T
  5.4849108606627643  1.3575316072750017 19.5548297969026130   T   T   T
 -0.0052636982217761  0.0000000000000010 19.1934403558584492   T   T   T
  3.3831219360157494  0.0000000000000012 20.7354661004020073   T   T   T
  1.2805333848359279  1.3575316072750017 19.5649733988598413   T   T   T
  6.7876580363750030  1.3575316072750010  9.2861208469999994   F   F   F
  6.7876580363750030  0.0000000000000004  8.0000000000000000   F   F   F
  8.8527351173617319  1.3575316072750010  9.2861208469999994   F   F   F
 10.1814870545625027  0.0000000000000005  9.2861208469999994   F   F   F
 10.1814870545625027  1.3575316072750012 12.5708101129999967   F   F   F
 10.1814870545625027  0.0000000000000006 11.2846892659999973   F   F   F
  6.7876580363750030  0.0000000000000006 10.5722416940000006   F   F   F
 11.5102389917632735  1.3575316072750010  9.2861208469999994   F   F   F
 12.2465641355492352  1.3575316072750012 12.5708101129999967   F   F   F
  6.7876580363750030  0.0000000000000007 12.5708101129999967   F   F   F
  6.6801215933092779  1.3575316072750012 15.9172690519470788   T   T   T
  6.7860461705535062  0.0000000000000009 14.6472429473069834   T   T   T
 10.1814870545625027  0.0000000000000008 13.8569309599999961   F   F   F
  8.1164099735757738  1.3575316072750012 12.5708101129999967   F   F   F
  8.8060415570301842  1.3575316072750012 15.9585146939675742   T   T   T
 10.1212659348530973  0.0000000000000009 16.1115358237721189   T   T   T
 10.1797796651980583  1.3575316072750017 19.5219233062931430   T   T   T
 10.1610088290522018  0.0000000000000010 18.0272541988943757   T   T   T
```

```
  6.7859768515567902  0.0000000000000010 17.3286977827209192   T   T   T
 11.5242574789913270  1.3575316072750012 15.9602554642624614   T   T   T
 12.2728170103954408  1.3575316072750017 19.5549320697160702   T   T   T
  6.7822056943016911  0.0000000000000011 19.1935639997223326   T   T   T
 10.1707311378759186  0.0000000000000011 20.7355348819754965   T   T   T
  8.0680201431950831  1.3575316072750017 19.5650752830417431   T   T   T

Metal reference: TiO2(110)/fcc(100)_5x1/Ir E_tot= -125.91286103 eV
 D3-zero damping= -6.2022427 eV, D3-BJ damping= -6.7226702 eV
Ir
 1.0000000000000000
    13.5753160727500024    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7150632145500007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7815818092786628
  15
Cartesian
  0.6738772458884220  0.0000000000000001  8.0398800826631973
  2.0313519690126984  1.3575316249809122  9.8941499358110132
  0.6734142335239420  0.0000000000000000 11.7479214983872353
  3.3892493191124555  0.0000000000000001  8.0403818622671253
  4.7469991461400411  1.3575316072750003  9.8942857113413645
  3.3894000931982573 -0.0000000000000001 11.7472468129544652
  6.1045368612454398  0.0000000000000000  8.0401301113021830
  7.4621318562818804  1.3575316072750003  9.8939892779118335
  6.1054437206078207 -0.0000000000000000 11.7479732646001569
  8.8195916472060567 -0.0000000000000000  8.0402341064210354
 10.1769437242045857  1.3575316072750003  9.8942389196321940
  8.8193206002191697  0.0000000000000000 11.7477400541039803
 11.5341455675291975 -0.0000000000000000  8.0402429256968766
 12.8918457575430878  1.3575316072750003  9.8939293182570349
 11.5344363125154477 -0.0000000000000000 11.7476230462646978

Interface: TiO2(110)/fcc(100)_5x1/Rh E_tot= -526.42309971 eV
 D3-zero damping= -15.0961282 eV, D3-BJ damping= -18.612818 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Rh
 1.0000000000000000
    13.3883134764000005    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.6776626952800004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.2949304730746931
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000007  1.3388313476400009  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  7.9999999999999991   F   F   F
  2.0366302460299690  1.3388313476400009  9.2861208469999994   F   F   F
  3.3470783691000010  0.0000000000000005  9.2861208469999994   F   F   F
  3.3470783691000010  1.3388313476400011 12.5708101129999967   F   F   F
  3.3470783691000010  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416939999988   F   F   F
  4.6575264921700334  1.3388313476400009  9.2861208469999994   F   F   F
  5.3837086151299687  1.3388313476400011 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 13.3898906809630240  1.3388313476400011 15.9619130302615009   T   T   T
  0.0008997766379345  0.0000000000000011 14.6420910749366975   T   T   T
  3.3470783691000010  0.0000000000000008 13.8569309599999961   F   F   F
  1.3104481230700329  1.3388313476400011 12.5708101129999967   F   F   F
  1.9915428091045209  1.3388313476400011 15.9681125147598344   T   T   T
  3.3482309478465018  0.0000000000000005 15.9860828551830281   T   T   T
  3.3459327984937826  1.3388313476400016 19.4059943598832021   T   T   T
  3.3477498685973379  0.0000000000000010 18.0073239368591125   T   T   T
 13.3903947891225581  0.0000000000000009 17.4179340667010969   T   T   T
  4.7028845328024795  1.3388313476400011 15.9445766574174499   T   T   T
```

```
  5.3903180833166404  1.3388313476400016 19.4869875381703501   T   T   T
  0.0057359864184674  0.0000000000000011 19.2866559462190352   T   T   T
  3.5690283217734828  0.0000000000000012 20.7881266715393949   T   T   T
  1.3464023202403419  1.3388313476400016 19.6383491634161054   T   T   T
  6.6941567382000020  1.3388313476400009  9.2861208469999994   F   F   F
  6.6941567382000020  0.0000000000000004  7.9999999999999991   F   F   F
  8.7307869842299688  1.3388313476400009  9.2861208469999994   F   F   F
 10.0412351073000021  0.0000000000000005  9.2861208469999994   F   F   F
 10.0412351073000021  1.3388313476400011 12.5708101129999967   F   F   F
 10.0412351073000021  0.0000000000000006 11.2846892659999973   F   F   F
  6.6941567382000020  0.0000000000000006 10.5722416939999988   F   F   F
 11.3516832303700337  1.3388313476400009  9.2861208469999994   F   F   F
 12.0778653533299707  1.3388313476400011 12.5708101129999967   F   F   F
  6.6941567382000020  0.0000000000000007 12.5708101129999967   F   F   F
  6.6954333712692629  1.3388313476400011 15.9125604665464611   T   T   T
  6.6993859097594353  0.0000000000000009 14.6041319974210744   T   T   T
 10.0412351073000021  0.0000000000000008 13.8569309599999961   F   F   F
  8.0046048612700336  1.3388313476400011 12.5708101129999967   F   F   F
  8.6905439006182892  1.3388313476400011 15.9548786514110201   T   T   T
 10.0445068581167263  0.0000000000000009 15.9923672725757147   T   T   T
 10.0558032909348327  1.3388313476400016 19.4145484296796411   T   T   T
 10.0563795725009193  0.0000000000000010 18.0163129280340080   T   T   T
  6.6940514197003305  0.0000000000000010 17.3272300541663391   T   T   T
 11.4004249651821805  1.3388313476400011 15.9687389669157476   T   T   T
 12.0544047244335086  1.3388313476400016 19.6438077123747092   T   T   T
  6.7017431052002454  0.0000000000000010 19.1916011404144413   T   T   T
  9.8276826870078811 -0.0000000124306627 20.8067801730764543   T   T   T
  8.0157392676199244  1.3388313476400016 19.4806533751085986   T   T   T
  0.0430802022810440  0.0000000000000000 22.6025704330198245   T   T   T
  1.3748094770324568  1.3388313476400002 24.4537403212011704   T   T   T
  0.0380194232554866  0.0000000000000000 26.3085880389110258   T   T   T
  2.5964055511858590  0.0000000000000000 22.5667039609207016   T   T   T
  4.0606087523874468  1.3388313476400002 24.3206866369590102   T   T   T
  2.7881029378166069  0.0000000000000000 26.2116172130304754   T   T   T
  5.3454392703951150  0.0000000000000000 22.3593931948788196   T   T   T
  6.7333628203882956  1.3388313476400002 24.1496736327254276   T   T   T
  5.4474997818966120  0.0000000000000000 26.0764149452219485   T   T   T
  8.1137453142369456 -0.0000000000000000 22.3554410540157171   T   T   T
  9.4106354552006071  1.3388313476400002 24.3085926437504405   T   T   T
  8.0256529263350842  0.0000000000000000 26.0671995184904048   T   T   T
 10.8796069628925185  0.0000000000000000 22.5517909714099147   T   T   T
 12.0949938847311120  1.3388313476400002 24.4472908432500695   T   T   T
 10.6767865659261840  0.0000000000000000 26.2020942280878835   T   T   T

Oxide reference: TiO2(110)/fcc(100)_5x1/Rh E_tot= -418.67995628 eV
 D3-zero damping= -7.250951 eV, D3-BJ damping= -10.3505455 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
    13.3883134764000005    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.6776626952800004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.8183887894624924
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000007  1.3388313476400009  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  8.0000000000000000   F   F   F
  2.0366302460299690  1.3388313476400009  9.2861208469999994   F   F   F
  3.3470783691000010  0.0000000000000005  9.2861208469999994   F   F   F
  3.3470783691000010  1.3388313476400011 12.5708101129999967   F   F   F
  3.3470783691000010  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416940000006   F   F   F
  4.6575264921700334  1.3388313476400009  9.2861208469999994   F   F   F
```

```
  5.3837086151299687  1.3388313476400011 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 13.3823715215590990  1.3388313476400011 15.9345206578445104   T   T   T
 -0.0060738822360059  0.0000000000000014 14.6501603257391295   T   T   T
  3.3470783691000010  0.0000000000000008 13.8569309599999961   F   F   F
  1.3104481230700329  1.3388313476400011 12.5708101129999967   F   F   F
  1.9901137135808558  1.3388313476400011 15.9797564519520972   T   T   T
  3.3405664362421255  0.0000000000000006 16.1640807615044046   T   T   T
  3.3372046027836015  1.3388313476400016 19.5896448904426883   T   T   T
  3.3361622797483168  0.0000000000000011 18.0745751114711268   T   T   T
 13.3836217767414567  0.0000000000000009 17.3670305459013683   T   T   T
  4.6923422679626503  1.3388313476400011 15.9861915138986195   T   T   T
  5.4017472515800895  1.3388313476400016 19.6260816071782465   T   T   T
 -0.0087608390299797  0.0000000000000010 19.2252437800438045   T   T   T
  3.3374223866584729  0.0000000000000012 20.8187300023037629   T   T   T
  1.2731412153459232  1.3388313476400016 19.6296600775840488   T   T   T
  6.6941567382000020  1.3388313476400009  9.2861208469999994   F   F   F
  6.6941567382000020  0.0000000000000004  8.0000000000000000   F   F   F
  8.7307869842299688  1.3388313476400009  9.2861208469999994   F   F   F
 10.0412351073000021  0.0000000000000005  9.2861208469999994   F   F   F
 10.0412351073000021  1.3388313476400011 12.5708101129999967   F   F   F
 10.0412351073000021  0.0000000000000006 11.2846892659999973   F   F   F
  6.6941567382000020  0.0000000000000006 10.5722416940000006   F   F   F
 11.3516832303700337  1.3388313476400009  9.2861208469999994   F   F   F
 12.0778653533299707  1.3388313476400011 12.5708101129999967   F   F   F
  6.6941567382000020  0.0000000000000007 12.5708101129999967   F   F   F
  6.6883284684766631  1.3388313476400011 15.9355258737811454   T   T   T
  6.6876605554775894  0.0000000000000009 14.6511575136123415   T   T   T
 10.0412351073000021  0.0000000000000008 13.8569309599999961   F   F   F
  8.0046048612700336  1.3388313476400011 12.5708101129999967   F   F   F
  8.6841921408667417  1.3388313476400011 15.9796604914819014   T   T   T
 10.0348318704753225  0.0000000000000009 16.1633034778642184   T   T   T
 10.0313626623552405  1.3388313476400016 19.5887225215347094   T   T   T
 10.0303356316364720  0.0000000000000010 18.0736704456327750   T   T   T
  6.6898685744390711  0.0000000000000010 17.3686192617857245   T   T   T
 11.3865252116590856  1.3388313476400011 15.9846839577719741   T   T   T
 12.0956406012046518  1.3388313476400016 19.6234479628734952   T   T   T
  6.6855551299891163  0.0000000000000010 19.2268536156948961   T   T   T
 10.0338259592490004  0.0000000000000011 20.8178158652424763   T   T   T
  7.9676317970035138  1.3388313476400016 19.6310916420723771   T   T   T

Metal reference: TiO2(110)/fcc(100)_5x1/Rh E_tot= -103.61599597 eV
 D3-zero damping= -5.0105634 eV, D3-BJ damping= -6.0426217 eV
Rh
 1.0000000000000000
    13.3883134764000005    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.6776626952800004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9690210088066564
  15
Cartesian
  0.0397744627602941  0.0000000000000003  8.1455670613964113
  1.3783564824865626  1.3388313476400002  9.9868800808567482
  0.0403509415442953  0.0000000000000000 11.8290578117650647
  2.7174321723854682  0.0000000000000000  8.1449384272022698
  4.0561826225905984  1.3388313476400002  9.9865170557893048
  2.7177709866194246  0.0000000000000000 11.8277531075729261
  5.3952464870821517  0.0000000000000000  8.1445360663562543
  6.7336973233696877  1.3388313815245776  9.9867242589492964
  5.3954717736336333 -0.0000000000000000 11.8279990601330631
  8.0722721297990496 -0.0000000000000000  8.1451835288054610
  9.4113954195581311  1.3388313707590664  9.9867863112123008
  8.0725735826955010 -0.0000000904229017 11.8280604977159971
 10.7506066319605971  0.0000000000000000  8.1457818332183187
```

```
 12.0892244707273591  1.3388313476400002  9.9876194848112263
 10.7499357242902853  0.0000000000000000 11.8276920159522145

Interface: TiO2(110)/fcc(100)_5x1/Os E_tot= -579.12624571 eV
 D3-zero damping= -13.8897933 eV, D3-BJ damping= -18.0838734 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Os
 1.0000000000000000
    13.5420714154000024    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7084142830800007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.3341849367763245
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000007  1.3542071415400010  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  7.9999999999999991   F   F   F
  2.0600199037106495  1.3542071415400010  9.2861208469999994   F   F   F
  3.3855178538500015  0.0000000000000005  9.2861208469999994   F   F   F
  3.3855178538500015  1.3542071415400012 12.5708101129999967   F   F   F
  3.3855178538500015  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416939999988   F   F   F
  4.7110158039893539  1.3542071415400010  9.2861208469999994   F   F   F
  5.4455377575606496  1.3542071415400012 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 13.5530897170589917  1.3542071415400012 15.9403141681901328   T   T   T
 -0.0204993434724548  0.0000000000000008 14.6338154017153155   T   T   T
  3.3855178538500015  0.0000000000000008 13.8569309599999961   F   F   F
  1.3254979501393529  1.3542071415400012 12.5708101129999967   F   F   F
  2.0196669192743859  1.3542071415400012 15.9229393529113743   T   T   T
  3.3876483325472697  0.0000000000000008 15.9088706176331289   T   T   T
  3.3841922022377129  1.3542071415400017 19.2826536697677682   T   T   T
  3.3851569459638711  0.0000000000000014 17.9279771438582891   T   T   T
 13.5432323298050488  0.0000000000000009 17.3629576402565107   T   T   T
  4.7537367250321960  1.3542071415400012 15.9232751895192806   T   T   T
  5.4463026090196491  1.3542071415400017 19.5028647446521006   T   T   T
 -0.0141623883921471  0.0000000000000010 19.2444289463808289   T   T   T
  3.3846742349178616  0.0000000000000011 20.6512558481374953   T   T   T
  1.3232033076064791  1.3542071415400017 19.5032117068456508   T   T   T
  6.7710357077000030  1.3542071415400010  9.2861208469999994   F   F   F
  6.7710357077000030  0.0000000000000004  7.9999999999999991   F   F   F
  8.8310556114106493  1.3542071415400010  9.2861208469999994   F   F   F
 10.1565535615500036  0.0000000000000005  9.2861208469999994   F   F   F
 10.1565535615500036  1.3542071415400012 12.5708101129999967   F   F   F
 10.1565535615500036  0.0000000000000006 11.2846892659999973   F   F   F
  6.7710357077000030  0.0000000000000006 10.5722416939999988   F   F   F
 11.4820515116893542  1.3542071415400010  9.2861208469999994   F   F   F
 12.2165734652606535  1.3542071415400012 12.5708101129999967   F   F   F
  6.7710357077000030  0.0000000000000007 12.5708101129999967   F   F   F
  6.7675644692110719  1.3542071415400012 15.9403703220380013   T   T   T
  6.7924572327384878  0.0000000000000009 14.6337423717763357   T   T   T
 10.1565535615500036  0.0000000000000008 13.8569309599999961   F   F   F
  8.0965336578393554  1.3542071415400012 12.5708101129999967   F   F   F
  8.8021576666971111  1.3542071415400012 15.9810644662820227   T   T   T
 10.1586279778720989  0.0000000000000009 15.9864199405281298   T   T   T
 10.1559672384985404  1.3542071415400017 19.4231785900275113   T   T   T
 10.1560359667198075  0.0000000000000010 18.0525268177460916   T   T   T
  6.7710098701924455  0.0000000000000009 17.3629568061716384   T   T   T
 11.5129463228836908  1.3542071415400012 15.9815547203260717   T   T   T
 12.1750374508090538  1.3542071415400017 19.5343599874460097   T   T   T
  6.7837482841011907  0.0000000000000011 19.2446012737615781   T   T   T
 10.1545894986074856  0.0000000000000012 20.9562825727996298   T   T   T
  8.1363721951249630  1.3542071415400017 19.5346099656242416   T   T   T
  0.6252588190746500  0.0000000000000001 22.6152213136292026   T   T   T
```

```
  2.0474613446269121  1.3542071415400003 24.4466190389386462   T   T   T
  0.6649485469872272  0.0000000000000000 26.2974048647937195   T   T   T
  3.3811424375474401 -0.0000000000000000 22.6037443341779287   T   T   T
  4.7161144506016930  1.3542071415400003 24.4454392553659723   T   T   T
  3.3815225227408483  0.0000000000000000 26.3197319127143743   T   T   T
  6.1386090280084487  0.0000000000000000 22.6140257825207662   T   T   T
  7.4659828915525797  1.3542071415400003 24.4338030920294997   T   T   T
  6.0986377226793484  0.0000000000000000 26.2962645202615839   T   T   T
  8.6795225645242393 -0.0000000000000000 22.4938644586296057   T   T   T
 10.1529331868220449  1.3542071415400003 24.3472719713854211   T   T   T
  8.8157402228980679  0.0000000000000001 26.2398655862127761   T   T   T
 11.6277641755838452 -0.0000000000000000 22.4946459562613441   T   T   T
 12.8400562979022546  1.3542071415400003 24.4356993720228033   T   T   T
 11.4886903847645314  0.0000000000000000 26.2408365252621181   T   T   T

Oxide reference: TiO2(110)/fcc(100)_5x1/Os E_tot= -420.51212845 eV
 D3-zero damping= -7.1314075 eV, D3-BJ damping= -10.1429062 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
    13.5420714154000024    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7084142830800007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.7535928717466120
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000007  1.3542071415400010  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  8.0000000000000000   F   F   F
  2.0600199037106495  1.3542071415400010  9.2861208469999994   F   F   F
  3.3855178538500015  0.0000000000000005  9.2861208469999994   F   F   F
  3.3855178538500015  1.3542071415400012 12.5708101129999967   F   F   F
  3.3855178538500015  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416940000006   F   F   F
  4.7110158039893539  1.3542071415400010  9.2861208469999994   F   F   F
  5.4455377575606496  1.3542071415400012 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 13.4513387709374204  1.3542071415400012 15.9220183319867452   T   T   T
 -0.0029118868726674  0.0000000000000010 14.6491764139149563   T   T   T
  3.3855178538500015  0.0000000000000008 13.8569309599999961   F   F   F
  1.3254979501393529  1.3542071415400012 12.5708101129999967   F   F   F
  2.0085306330371595  1.3542071415400012 15.9661127896533444   T   T   T
  3.3318489649218606  0.0000000000000005 16.1227129262599433   T   T   T
  3.3804720891727889  1.3542071415400017 19.5364067947048952   T   T   T
  3.3661890204327576  0.0000000000000011 18.0374551066204809   T   T   T
 13.5380947900341351  0.0000000000000009 17.3376625452413791   T   T   T
  4.7252197384083185  1.3542071415400012 15.9669181124609523   T   T   T
  5.4696294267297745  1.3542071415400017 19.5691313111986105   T   T   T
 -0.0073666980066512  0.0000000000000010 19.2011294684781006   T   T   T
  3.3757199982558497  0.0000000000000012 20.7528038089797313   T   T   T
  1.2786063641454155  1.3542071415400017 19.5780578838186905   T   T   T
  6.7710357077000030  1.3542071415400010  9.2861208469999994   F   F   F
  6.7710357077000030  0.0000000000000004  8.0000000000000000   F   F   F
  8.8310556114106493  1.3542071415400010  9.2861208469999994   F   F   F
 10.1565535615500036  0.0000000000000005  9.2861208469999994   F   F   F
 10.1565535615500036  1.3542071415400012 12.5708101129999967   F   F   F
 10.1565535615500036  0.0000000000000006 11.2846892659999973   F   F   F
  6.7710357077000030  0.0000000000000006 10.5722416940000006   F   F   F
 11.4820515116893542  1.3542071415400010  9.2861208469999994   F   F   F
 12.2165734652606535  1.3542071415400012 12.5708101129999967   F   F   F
  6.7710357077000030  0.0000000000000007 12.5708101129999967   F   F   F
  6.6803649875709716  1.3542071415400012 15.9220296020861323   T   T   T
  6.7677142645028967  0.0000000000000009 14.6491534901289828   T   T   T
 10.1565535615500036  0.0000000000000008 13.8569309599999961   F   F   F
```

```
  8.0965336578393554  1.3542071415400012 12.5708101129999967   F   F   F
  8.7796480467943638  1.3542071415400012 15.9658949762821702   T   T   T
 10.1029071955114667  0.0000000000000009 16.1228793876785765   T   T   T
 10.1516605635013999  1.3542071415400017 19.5365426669616937   T   T   T
 10.1373063523410458  0.0000000000000010 18.0375186401586873   T   T   T
  6.7672660231401869  0.0000000000000010 17.3376737466692070   T   T   T
 11.4963169566547112  1.3542071415400012 15.9668677299391657   T   T   T
 12.2405750801041115  1.3542071415400017 19.5692116569545789   T   T   T
  6.7637260426046826  0.0000000000000011 19.2012330252185919   T   T   T
 10.1467869574555127  0.0000000000000011 20.7529291550619455   T   T   T
  8.0497926417694021  1.3542071415400017 19.5778622980147681   T   T   T

Metal reference: TiO2(110)/fcc(100)_5x1/Os E_tot= -154.53045022 eV
 D3-zero damping= -4.818198 eV, D3-BJ damping= -5.7753607 eV
Os
 1.0000000000000000
    13.5420714154000024    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.7084142830800007    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.8641864034588842
  15
Cartesian
  0.6740899330126008  0.0000000000000000  8.1019742346460912
  2.0283019915887603  1.3542071415400003  9.9539592669845138
  0.6735847309107378  0.0000000000000000 11.8057222565139419
  3.3820326128736471 -0.0000000000000000  8.1018813258381179
  4.7361774821375153  1.3542071415400003  9.9536808615935470
  3.3824104893004767  0.0000000000000000 11.8057667735043417
  6.0899683840623329  0.0000000000000000  8.1018105631001678
  7.4447788361276208  1.3542071415400003  9.9529822907431189
  6.0912917587864062  0.0000000000000000 11.8055000570321660
  8.7990794783710911 -0.0000000000000000  8.1013181227996132
 10.1531330055237756  1.3542071415400003  9.9531534301069762
  8.7988824653458622  0.0000000000000001 11.8049757087892573
 11.5077152370927340 -0.0000000000000000  8.1015107308387719
 12.8616155041820068  1.3542070862520241  9.9538552354249035
 11.5071990807012003  0.0000000000000000 11.8051252206173896

Interface: TiO2(110)/fcc(100)_5x1/Ru E_tot= -550.77642369 eV
 D3-zero damping= -14.8970079 eV, D3-BJ damping= -18.4030124 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ru
 1.0000000000000000
    13.3309737097000021    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.6661947419400005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   34.3341573543177745
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2  15
Selective dynamics
Cartesian
  0.0000000000000007  1.3330973709700009  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  8.0000000000000000   F   F   F
  2.0279077207195653  1.3330973709700009  9.2861208469999994   F   F   F
  3.3327434274250014  0.0000000000000005  9.2861208469999994   F   F   F
  3.3327434274250014  1.3330973709700011 12.5708101129999967   F   F   F
  3.3327434274250014  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416940000024   F   F   F
  4.6375791341304380  1.3330973709700009  9.2861208469999994   F   F   F
  5.3606511481445649  1.3330973709700011 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 13.3219759251392631  1.3330973097550818 15.9668108349687117   T   T   T
 -0.0136494908185639 -0.0000000354509550 14.6396859077585013   T   T   T
  3.3327434274250014  0.0000000000000008 13.8569309599999961   F   F   F
  1.3048357067054368  1.3330973709700011 12.5708101129999967   F   F   F
  1.9671645029723959  1.3330973709700011 15.9640182738369010   T   T   T
```

```
  3.3201240073611360  0.0000000000000004 15.9923125156101520   T   T   T
  3.2857542184548265  1.3330971630511046 19.4273913657636612   T   T   T
  3.2764894067730563 -0.0000001271162938 18.0301603364037213   T   T   T
 13.3297808943802085 -0.0000000928638531 17.4313560945227692   T   T   T
  4.6732150021539409  1.3330973709700011 15.9782996373081954   T   T   T
  5.3136557629361079  1.3330972659001823 19.4706310624027488   T   T   T
 -0.0311125437849159 -0.0000001600963860 19.2942096276148440   T   T   T
  3.5623701590533834 -0.0000001743046056 20.8665804364926863   T   T   T
  1.3109878705229168  1.3330972272849777 19.7012963831496357   T   T   T
  6.6654868548500028  1.3330973709700009  9.2861208469999994   F   F   F
  6.6654868548500028  0.0000000000000004  8.0000000000000000   F   F   F
  8.6933945755695650  1.3330973709700009  9.2861208469999994   F   F   F
  9.9982302822750011  0.0000000000000005  9.2861208469999994   F   F   F
  9.9982302822750011  1.3330973709700011 12.5708101129999967   F   F   F
  9.9982302822750011  0.0000000000000006 11.2846892659999973   F   F   F
  6.6654868548500028  0.0000000000000006 10.5722416940000024   F   F   F
 11.3030659889804372  1.3330973709700009  9.2861208469999994   F   F   F
 12.0261380029945677  1.3330973709700011 12.5708101129999967   F   F   F
  6.6654868548500028  0.0000000000000007 12.5708101129999967   F   F   F
  6.6565738117850950  1.3330973960088719 15.9146806370287415   T   T   T
  6.6474131543923285 -0.0000000103937459 14.6003904578202395   T   T   T
  9.9982302822750011  0.0000000000000008 13.8569309599999961   F   F   F
  7.9703225615554381  1.3330973709700011 12.5708101129999967   F   F   F
  8.6369483266213560  1.3330973709700011 15.9395984497825864   T   T   T
  9.9887117218300467  0.0000000000000008 15.9761621653319708   T   T   T
  9.9713020890293773  1.3330972815122610 19.4062237713616987   T   T   T
  9.9697756256050507 -0.0000000287625447 18.0132946783893395   T   T   T
  6.6706067939071483 -0.0000000425638927 17.3364431500802887   T   T   T
 11.3436905141705449  1.3330973709700011 15.9862486764711793   T   T   T
 11.9488587856526873  1.3330972525492590 19.6484233093912231   T   T   T
  6.6341744305501420 -0.0000000777253057 19.1937864123073219   T   T   T
  9.7565590968265123 -0.0000000414822423 20.8561923137550203   T   T   T
  7.9497752038845002  1.3330973224277962 19.5188964878359599   T   T   T
  0.0469416146561826  0.0000011743121389 22.6604670522991327   T   T   T
  1.3982506256039828  1.3330975546147541 24.5242997056378975   T   T   T
  0.0041481419508450 -0.0000001049048134 26.3249689738906874   T   T   T
  2.5541211864744686 -0.0000003060745888 22.6133293659095713   T   T   T
  4.0345562113793596  1.3330973251268068 24.3653428142122301   T   T   T
  2.7677309862457515  0.0000001288537695 26.2444058718539104   T   T   T
  5.2349402969339947 -0.0000001224298355 22.3552389173822057   T   T   T
  6.6916390145782421  1.3330974321849196 23.9796801726732802   T   T   T
  5.4800976957996532 -0.0000002213113048 26.0550591374358582   T   T   T
  8.1365355447058576 -0.0000000000000000 22.3524143724252973   T   T   T
  9.3654165960606317  1.3330975922813055 24.3161702678791798   T   T   T
  7.9446710422102917 -0.0000001224298355 26.0358331798290301   T   T   T
 10.8553406825672489  0.0000003014869199 22.5569155689947536   T   T   T
 11.9973128462920560  1.3330984166708288 24.4607665474444858   T   T   T
 10.6533789320861256  0.0000007041144939 26.2122290272097729   T   T   T

Oxide reference: TiO2(110)/fcc(100)_5x1/Ru E_tot= -417.82755781 eV
 D3-zero damping= -7.2954413 eV, D3-BJ damping= -10.4261593 eV
Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O Ti  O
 1.0000000000000000
    13.3309737097000021    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.6661947419400005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   28.8489296042885357
   1   2   2   4   2   4   2   4   1   2   1   2   2   4   2   4   2   4
1   2
Selective dynamics
Cartesian
  0.0000000000000007  1.3330973709700009  9.2861208469999994   F   F   F
  0.0000000000000005  0.0000000000000004  8.0000000000000000   F   F   F
  2.0279077207195653  1.3330973709700009  9.2861208469999994   F   F   F
```

```
  3.3327434274250014  0.0000000000000005  9.2861208469999994   F   F   F
  3.3327434274250014  1.3330973709700011 12.5708101129999967   F   F   F
  3.3327434274250014  0.0000000000000006 11.2846892659999973   F   F   F
  0.0000000000000007  0.0000000000000006 10.5722416940000006   F   F   F
  4.6375791341304380  1.3330973709700009  9.2861208469999994   F   F   F
  5.3606511481445649  1.3330973709700011 12.5708101129999967   F   F   F
  0.0000000000000008  0.0000000000000007 12.5708101129999967   F   F   F
 13.3052751741916016  1.3330973709700011 15.9399862698405617   T   T   T
 -0.0186431664294444  0.0000000000000011 14.6521986738639818   T   T   T
  3.3327434274250014  0.0000000000000008 13.8569309599999961   F   F   F
  1.3048357067054368  1.3330973709700011 12.5708101129999967   F   F   F
  1.9662356089562814  1.3330973709700011 15.9833219955843759   T   T   T
  3.3090767876667768  0.0000000000000005 16.1864110540356165   T   T   T
  3.3003460730986265  1.3330973709700016 19.6160545632011178   T   T   T
  3.2980849782283412  0.0000000000000011 18.0939421640997651   T   T   T
 13.3188457560931166  0.0000000000000010 17.3798088845115721   T   T   T
  4.6607528597143020  1.3330973709700011 16.0012181084781062   T   T   T
  5.3555166412498565  1.3330973709700016 19.6393979368461977   T   T   T
 -0.0277087471273805  0.0000000000000011 19.2356537445388867   T   T   T
  3.3094587138739491  0.0000000000000012 20.8496652819698411   T   T   T
  1.2493683104567070  1.3330973709700016 19.6605458633718797   T   T   T
  6.6654868548500028  1.3330973709700009  9.2861208469999994   F   F   F
  6.6654868548500028  0.0000000000000004  8.0000000000000000   F   F   F
  8.6933945755695650  1.3330973709700009  9.2861208469999994   F   F   F
  9.9982302822750011  0.0000000000000005  9.2861208469999994   F   F   F
  9.9982302822750011  1.3330973709700011 12.5708101129999967   F   F   F
  9.9982302822750011  0.0000000000000006 11.2846892659999973   F   F   F
  6.6654868548500028  0.0000000000000006 10.5722416940000006   F   F   F
 11.3030659889804372  1.3330973709700009  9.2861208469999994   F   F   F
 12.0261380029945677  1.3330973709700011 12.5708101129999967   F   F   F
  6.6654868548500028  0.0000000000000007 12.5708101129999967   F   F   F
  6.6399202475631345  1.3330973709700011 15.9394582082532938   T   T   T
  6.6469534028392347  0.0000000000000008 14.6517343379206260   T   T   T
  9.9982302822750011  0.0000000000000008 13.8569309599999961   F   F   F
  7.9703225615554381  1.3330973709700011 12.5708101129999967   F   F   F
  8.6317719794235366  1.3330973709700011 15.9831851343914444   T   T   T
  9.9744764411631621  0.0000000000000009 16.1867820289840587   T   T   T
  9.9660006497864337  1.3330973709700016 19.6164544798594527   T   T   T
  9.9635619546893341  0.0000000000000010 18.0942483949289716   T   T   T
  6.6538324077419979  0.0000000000000009 17.3791636526097051   T   T   T
 11.3260527284453865  1.3330973709700011 16.0012760215899412   T   T   T
 12.0208989309915193  1.3330973709700016 19.6401191172963827   T   T   T
  6.6379260080714442  0.0000000000000011 19.2350183092871987   T   T   T
  9.9749768545033213  0.0000000000000011 20.8500630478371214   T   T   T
  7.9149402472872739  1.3330973709700016 19.6602310806493321   T   T   T

Metal reference: TiO2(110)/fcc(100)_5x1/Ru E_tot= -128.11217152 eV
 D3-zero damping= -4.734037 eV, D3-BJ damping= -5.7740992 eV
Ru
 1.0000000000000000
    13.3309737097000021    0.0000000000000000    0.0000000000000000
     0.0000000000000000    2.6661947419400005    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.1501239330877873
  15
Cartesian
  0.0488316478661278 -0.0000001772096682  8.2621987573661801
  1.3754279929114379  1.3330973709700003 10.1038644620238216
  0.0357731467305247 -0.0000000000000000 11.9195138144240520
  2.7025117221305224  0.0000001772096681  8.2631596778303962
  4.0415758796274135  1.3330973709700003 10.0942299279212957
  2.7129474797295345  0.0000000000000000 11.9211880413662890
  5.3586884573217928 -0.0000000000000000  8.2449882865784403
  6.7071353934344069  1.3330973709700003 10.0502185316488788
```

```
  5.3908665492565921  0.0000000000000000 11.9043731523922371
  8.0421895723964720  0.0000000000000000  8.2319977511035241
  9.3738227549443600  1.3330973709700003 10.0553756582260885
  8.0409382566351120 -0.0000000000000000 11.8917625032239496
 10.7222059074685010  0.0000000000000000  8.2450130336595748
 12.0400685025849690  1.3330975481796721 10.0917905844266187
 10.6924808946739791  0.0000000000000000 11.9053819341588287
```

Structures for calculating the adhesion with adjusting the metal to the oxide lattice constant

```
Interface with oxide lattice constant: O-a-SiO2(0001)/fcc(111)_2x2/Cu
E_tot= -275.50674245 eV
 D3-zero damping= -9.0274355 eV, D3-BJ damping= -11.3171833 eV
Si  O Si  O Si  O  H Cu
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999987    4.2975558034858610    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.5108124600182009
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.5589578055641859  0.1835607425578427  9.0169746245084834   F   F   F
 -1.2460063245427062  2.3706020739380591 10.8612336967246375   F   F   F
  2.2954873726859053  2.6196387297796453 11.6081185941916676   F   F   F
  3.4828408076011028  1.4113732975935680  9.5654178022134726   F   F   F
 -0.6270092618390272  3.7596400629834141 10.2987723773365918   F   F   F
  1.1042088912653403  3.4333422918536534  8.2518078419286898   F   F   F
 -0.1950063026963111  1.7174372615560012 11.9218080039603880   F   F   F
  2.6069757309659334 -0.0448243720647175 14.5050718430130114   F   F   F
  1.2211146816757126  2.0103212146560763 12.6701466762358965   F   F   F
 -1.3519408543316325  2.2463077618145353 16.3195406015923545   T   T   T
  2.1461463688185192  2.4639375497671381 16.9706042640287542   T   T   T
  3.5623960111059301  1.0817024797293637 15.1823391586074923   T   T   T
  1.7363447519784174  0.6009253703169686 13.2917821082657621   F   F   F
 -0.8760441044179764  3.6439872374616753 15.6339921134246538   T   T   T
  1.0572083999651556  3.0745478039444145 13.8903255655927058   F   F   F
 -0.3326907949751182  1.8190543995462924 17.5063150339052065   T   T   T
 -0.0930237020429611  4.3275272322148579 20.0248280933962413   T   T   T
  1.0820381276062816  2.2558625187551224 18.1741778038025892   T   T   T
  3.7754591320608175  2.1145436733778005 21.8491497483670543   T   T   T
  3.2107264414142818  0.7066407560074022 21.2504740457618269   T   T   T
  1.4816584522390690  1.1101451611319240 19.2392426738742977   T   T   T
 -1.0745043488219346  3.1780932153486274 20.6236117743807945   T   T   T
  0.9483140254809278  3.6665615071403725 18.9673023682092996   T   T   T
  0.2140622008885754  1.8755769797304414 22.6418311595344939   T   T   T
  2.7111862745694659  2.6844580289190807 22.9772730847675959   T   T   T
  1.3773667780178473  0.6802549719477083  8.0000000000000018   F   F   F
  1.1764967236772887  1.6519932737523471  8.0158744918591101   F   F   F
  1.9734199373505092  3.8385033657559648  8.0308754104330919   F   F   F
  6.1855742655713524 -0.8626994301013983 24.5093249320669493   T   T   T
  4.9195270255850980 -0.1818818457113323 26.4897586554882807   T   T   T
  4.9349751725452018 -1.6077552036679410 28.5760490462541199   T   T   T
  6.1785958954035847 -0.8886604024032484 30.6804430079823653   T   T   T
  3.5933452966329051 -0.9171737502727666 23.9785645399050829   T   T   T
  2.4758965709046779 -0.1806807041467054 26.4330663515865965   T   T   T
  2.4620095878295265 -1.6015289549732137 28.5731140035374800   T   T   T
  3.6962499600064445 -0.8905870284475879 30.6946855004509551   T   T   T
  4.9127323737126929  1.1938816277129287 24.4575100270361716   T   T   T
  3.6993494215388201  1.9629105610550910 26.5286251724407975   T   T   T
  3.6953093084205606  0.5355169775100393 28.5853419301178313   T   T   T
  4.9365656223215844  1.2587398813757382 30.6709047976811426   T   T   T
```

```
  2.4521729171267603  1.2381551025573059 24.4297968950043725   T   T   T
  1.2154196195818847  1.9821734189294840 26.4716945452647607   T   T   T
  1.2209751036585361  0.5391907047614701 28.5648962408860392   T   T   T
  2.4545779608853682  1.2581477774282650 30.6836254142405522   T   T   T

Metal reference with oxide lattice constant: O-a-SiO2(0001)/fcc(111)_2x2/Cu
E_tot= -61.77022633 eV
 D3-zero damping= -5.9946967 eV, D3-BJ damping= -7.2657742 eV
Cu
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999987    4.2975558034858610    0.0000000000000000
     0.0000000000000014    0.0000000000000024   22.5208294705541086
  16
Cartesian
  6.1609337699850082 -0.9676991827689199  8.2497503540808808
  4.9208293017575668 -0.2439138441738277 10.3627683832376256
  4.9198246341553675 -1.6664810603533649 12.4505127571860612
  6.1578110797332144 -0.9446874749548220 14.5627278571457577
  3.6789057497429969 -0.9686004087516470  8.2496546901101802
  2.4398472505084268 -0.2434290798190706 10.3626558914922082
  2.4386447797879782 -1.6665071068621244 12.4504808735556356
  3.6764517941219892 -0.9446466944691279 14.5621996344389792
  4.9202191976808267  1.1798235393751522  8.2493151482418021
  3.6805871478540317  1.9055276669612047 10.3617996725223716
  3.6790943612670866  0.4822260160858032 12.4498306113221471
  4.9170028520241074  1.2039691915192527 14.5626404135649139
  2.4394453360357806  1.1806152312371561  8.2493333168497394
  1.1993029122319820  1.9051144587404651 10.3622801212491211
  1.1980202786939147  0.4821378605620953 12.4513476211604601
  2.4360720547805128  1.2040288056387340 14.5624315145154188

Interface with oxide lattice constant: O-a-SiO2(0001)/fcc(111)_2x2/Pt
E_tot= -313.27751816 eV
 D3-zero damping= -12.7649322 eV, D3-BJ damping= -13.56282 eV
Si  O Si  O Si  O  H Pt
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999987    4.2975558034858610    0.0000000000000000
     0.0000000000000026    0.0000000000000045   42.4332323882753926
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.5589578055641864  0.1835607425578427  9.0169746245084816   F   F   F
 -1.2460063245427062  2.3706020739380596 10.8612336967246357   F   F   F
  2.2954873726859062  2.6196387297796457 11.6081185941916658   F   F   F
  3.4828408076011033  1.4113732975935680  9.5654178022134708   F   F   F
 -0.6270092618390271  3.7596400629834146 10.2987723773365900   F   F   F
  1.1042088912653409  3.4333422918536534  8.2518078419286880   F   F   F
 -0.1950063026963110  1.7174372615560012 11.9218080039603862   F   F   F
  2.6069757309659338 -0.0448243720647177 14.5050718430130097   F   F   F
  1.2211146816757126  2.0103212146560763 12.6701466762358947   F   F   F
 -1.3688993445393847  2.2535750485361552 16.3129206263744635   T   T   T
  2.1111425711968645  2.4981651846043702 16.9277800748459555   T   T   T
  3.5600800331783771  1.0900033267388267 15.1741645739555224   T   T   T
  1.7363447519784174  0.6009253703169685 13.2917821082657603   F   F   F
 -0.8672856549797645  3.6486611335164092 15.6441602430118909   T   T   T
  1.0572083999651558  3.0745478039444145 13.8903255655927040   F   F   F
 -0.3701154402003345  1.7993028011642924 17.5154128520577999   T   T   T
 -0.0828235322305391  4.1514041520436544 19.9829338639027405   T   T   T
  1.1099852567009241  2.0706657659738168 18.1349576832492829   T   T   T
  3.5242128679423739  2.1107230703289344 21.8617444654186386   T   T   T
  3.1230755966568577  0.7278973374360050 21.1273242670837078   T   T   T
```

```
  1.6166212922243448  0.7224583897746305 18.8642258075184159   T   T   T
 -1.1801102054773751  3.2114168411951365 20.7061606112266503   T   T   T
  1.0519209672093055  3.2635905471310718 19.2349315119067441   T   T   T
 -0.1406947721608349  1.8672366269541101 22.8299381956670153   T   T   T
  2.2834593979556845  2.6300745582297154 22.8099670144750206   T   T   T
  1.3773667780178476  0.6802549719477082  8.0000000000000000   F   F   F
  1.1764967236772892  1.6519932737523473  8.0158744918591083   F   F   F
  1.9734199373505097  3.8385033657559648  8.0308754104330902   F   F   F
  4.8310011000409077  0.0837083401642569 23.9379279068948208   T   T   T
  4.5081470470101506 -0.7631093740188065 27.1004800738893898   T   T   T
  4.5608832864500704 -0.0742906250185815 29.7034370535419221   T   T   T
  6.0795632892942031 -0.5284763869212178 33.5273682356016636   T   T   T
  2.3410354787378473 -0.6418489633611366 24.4033290858774023   T   T   T
  2.0783652016867067  0.1855208212861844 26.9283220753521633   T   T   T
  2.1250752135995712 -0.5456123726374226 30.2850552358722105   T   T   T
  3.5136496445383822 -0.3474292760333634 32.5459341151520576   T   T   T
  4.9559855828261936  1.5985843449851669 25.9663550805919563   T   T   T
  3.9274103009044641  2.1425821017554845 28.3132127845472041   T   T   T
  2.8679962700106461  2.0695785526565325 31.3379145465311701   T   T   T
  4.2572859164367491  1.3440716616095292 34.3627157494841100   T   T   T
  2.4422247627881255  1.9652740052854616 24.9386955874689313   T   T   T
  1.4441914503690956  1.6884637708916659 29.0134152304965234   T   T   T
  0.4093311249548883  1.4577112159734116 31.7459816855362362   T   T   T
  1.7704852811284726  1.9650639420475944 34.1608988003984138   T   T   T

Metal reference with oxide lattice constant: O-a-SiO2(0001)/fcc(111)_2x2/Pt
E_tot= -99.56674915 eV
 D3-zero damping= -9.4167918 eV, D3-BJ damping= -9.2942762 eV
Pt
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999987    4.2975558034858610    0.0000000000000000
     0.0000000000000014    0.0000000000000024   22.9261858102042275
  16
Cartesian
  6.4494501298076274 -0.9363007396506627  6.5704196898588991
  5.3503433438684880 -0.2394855190000800  9.9714232437946855
  4.5162292571802212 -1.4472228805497236 12.2091018894595891
  6.5462076588646045 -1.0415771187165321 16.0343503626006871
  3.9425455179251010 -0.6965992967249046  7.7406348070822215
  2.6742888442290225  0.4999373830738503 11.0610240913802098
  1.8125392021379430 -0.6089653223081279 13.2948009005198280
  3.9398819552092310 -1.1126238964092987 14.8500250125610513
  5.4589390090943040  1.3182662421835061  7.1561783926673055
  3.2198271527211282  1.7243950874530867  8.8026942557384587
  3.2825215946309494  1.3422964394170698 14.1787820120160699
  4.7054060733983887  0.7612529757652849 16.5347665573688651
  2.9168852631162787  1.1153732470458213  6.0925668840713341
  0.5995857633950772  2.4205255395888847  9.9190282675416110
  0.0177634587573063  1.1958316526690675 12.2609209105287125
  2.1994138044278437  1.4230802131074720 16.6322859584927834

Interface with oxide lattice constant: O-a-SiO2(0001)/fcc(111)_2x2/Ni
E_tot= -301.01859307 eV
 D3-zero damping= -7.3869579 eV, D3-BJ damping= -9.4788605 eV
Si  O  H Ni
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999983    4.2975558034858601    0.0000000000000000
     0.0000000000000023    0.0000000000000041   38.3240056714864323
   8  18   2  16
Selective dynamics
Cartesian
```

```
  2.5589578055641859  0.1835607425578427  9.0169746245084816   F   F   F
 -1.2460063245427058  2.3706020739380587 10.8612336967246357   F   F   F
  2.6069757309659334 -0.0448243720647175 14.5050718430130097   F   F   F
  1.2211146816757124  2.0103212146560758 12.6701466762358947   F   F   F
 -1.3709950360385654  2.2540523290472128 16.3128257974574815   T   T   T
 -0.1715236516562973  4.1266908581413624 19.9935211756641067   T   T   T
  1.0923707080173466  2.1192835417813889 18.1548609418448201   T   T   T
  3.6734327292302518  1.9607096919935272 21.7973933494384617   T   T   T
  2.2954873726859057  2.6196387297796444 11.6081185941916658   F   F   F
  3.4828408076011024  1.4113732975935678  9.5654178022134708   F   F   F
 -0.6270092618390267  3.7596400629834137 10.2987723773365900   F   F   F
  1.1042088912653405  3.4333422918536525  8.2518078419286880   F   F   F
 -0.1950063026963109  1.7174372615560010 11.9218080039603862   F   F   F
  2.1166993968190129  2.4773120215472813 16.9473251423092748   T   T   T
  3.5594632999694684  1.0879241701053373 15.1758847400916377   T   T   T
  1.7363447519784172  0.6009253703169685 13.2917821082657603   F   F   F
 -0.8784625705983181  3.6491605596077372 15.6354309635303039   T   T   T
  1.0572083999651556  3.0745478039444132 13.8903255655927040   F   F   F
 -0.3684228919003295  1.8169598218464713 17.5102387017161583   T   T   T
  2.9222866422346367  0.6261328154275547 21.2622208348165351   T   T   T
  1.5175708235598944  0.7946239496810207 18.9720023491911824   T   T   T
 -1.2099627776917865  3.0098903412709190 20.5612957187154919   T   T   T
  1.0220765475744489  3.3884213074889797 19.1701710324610346   T   T   T
  0.1433353829558653  1.6040867043263283 22.4612812861591138   T   T   T
  2.7379890465145338  2.6478051029081180 23.0240552584150571   T   T   T
  1.3773667780178471  0.6802549719477082  7.9999999999999991   F   F   F
  1.1764967236772887  1.6519932737523466  8.0158744918591047   F   F   F
  1.9734199373505092  3.8385033657559635  8.0308754104330866   F   F   F
  6.3964653460876963 -0.8535223798422227 24.3716289428728814   T   T   T
  5.1135872886818117 -0.1635384917771173 26.3322319789811665   T   T   T
  5.1090561675648027 -1.6065812792843039 28.3451430807398204   T   T   T
  6.3497200930068054 -0.8899885425117994 30.3329015032499747   T   T   T
  3.8704284824310866 -0.8728631201091809 24.2787089930960356   T   T   T
  2.6510969401009534 -0.1786632315410761 26.3169525660575623   T   T   T
  2.6293002658637477 -1.6065394105611028 28.3415349627933324   T   T   T
  3.8674506003198759 -0.8906497736764932 30.3349257138011126   T   T   T
  5.1356294794195705  1.2666495003500462 24.3004190100829405   T   T   T
  3.8816054857554336  1.9760600038231546 26.3638342720685301   T   T   T
  3.8706067927154071  0.5393504528080505 28.3392743076256686   T   T   T
  5.1095080013375540  1.2569880436117804 30.3442589516536785   T   T   T
  2.6477051307378350  1.2376406944785017 24.3885445137296699   T   T   T
  1.3870704840595498  1.9771702656374084 26.3456861341852324   T   T   T
  1.3902825055176518  0.5394051444878759 28.3292307694404570   T   T   T
  2.6272905964012341  1.2549094139028900 30.3336273924920441   T   T   T

Metal reference with oxide lattice constant: O-a-SiO2(0001)/fcc(111)_2x2/Ni
E_tot= -86.86 eV
 D3-zero damping= -4.4585852 eV, D3-BJ damping= -5.5394090 eV
Ni
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999983    4.2975558034858601    0.0000000000000000
     0.0000000000000013    0.0000000000000023   21.9895023968654719
  16
Cartesian
  6.3461583800391121 -0.8569484135493008  8.0022407106975244
  5.1060988805465648 -0.1366473961561881  9.9988046161289930
  5.1062089980502119 -1.5659160345008749 11.9910185732089634
  6.3449284242178017 -0.8531178261349177 13.9880745484325644
  3.8650631456280835 -0.8567997471559895  8.0022551001733913
  2.6249522277101858 -0.1366258288084214  9.9988107669984512
  2.6251600991198427 -1.5658603734725105 11.9909721209214233
  3.8637756846434446 -0.8531349926466230 13.9882749800298125
```

```
  5.1057164992657977  1.2918447450096591  8.0022956353511425
  3.8655006626086372  2.0122485946137987  9.9991335020051491
  3.8657102900032232  0.5828613789627436 11.9909395111454575
  5.1047243410586418  1.2959170835730214 13.9885916380991429
  2.6245770566212423  1.2918385927758345  8.0022806575813075
  1.3843402268880163  2.0120172194099881  9.9989904633789219
  1.3845736271267683  0.5828032558373339 11.9908253812600556
  2.6231886900099219  1.2957060275989654 13.9881189022557084

Interface with oxide lattice constant: O-a-SiO2(0001)/fcc(111)_2x2/Ir
E_tot= -354.51238247 eV
 D3-zero damping= -11.6749543 eV, D3-BJ damping= -12.9227468 eV
Si  O Si  O Si  O  H Ir
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999983    4.2975558034858610    0.0000000000000000
     0.0000000000000025    0.0000000000000044   41.5964494858950289
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.5589578055641864  0.1835607425578427  9.0169746245084816   F   F   F
 -1.2460063245427060  2.3706020739380591 10.8612336967246357   F   F   F
  2.2954873726859057  2.6196387297796453 11.6081185941916658   F   F   F
  3.4828408076011033  1.4113732975935680  9.5654178022134708   F   F   F
 -0.6270092618390269  3.7596400629834146 10.2987723773365900   F   F   F
  1.1042088912653407  3.4333422918536534  8.2518078419286880   F   F   F
 -0.1950063026963110  1.7174372615560012 11.9218080039603862   F   F   F
  2.6069757309659338 -0.0448243720647176 14.5050718430130097   F   F   F
  1.2211146816757126  2.0103212146560763 12.6701466762358947   F   F   F
 -1.3455901255622338  2.2397350899316817 16.3183969692538966   T   T   T
  2.1545211657503387  2.4519700057241871 16.9833709378023663   T   T   T
  3.5650221642988384  1.0856729601129023 15.1706140456769187   T   T   T
  1.7363447519784172  0.6009253703169686 13.2917821082657603   F   F   F
 -0.8690077416573990  3.6418702002743499 15.6422556258767305   T   T   T
  1.0572083999651558  3.0745478039444141 13.8903255655927040   F   F   F
 -0.3311633684415475  1.7863600946545235 17.4992565054477751   T   T   T
 -0.2076209434750161  3.9881167041848165 19.9747843118727815   T   T   T
  1.1266385676387276  2.0392478405808974 18.1686511207232613   T   T   T
  3.5453892154022282  1.8365777173745392 21.7608677118597420   T   T   T
  2.7065963393225863  0.5239088671029768 21.2992164201624732   T   T   T
  1.5302417059807729  0.6553076932838132 18.9088298742038390   T   T   T
 -1.1941629777997207  2.7889661883815076 20.4651847835370120   T   T   T
  1.0600746366004277  3.2778279148099081 19.2341233519282646   T   T   T
 -0.0029489502958737  1.3343063786869698 22.3879312459173185   T   T   T
  2.5953964960469076  2.7566205134257693 22.7952422907419141   T   T   T
  1.3773667780178473  0.6802549719477082  8.0000000000000000   F   F   F
  1.1764967236772890  1.6519932737523473  8.0158744918591083   F   F   F
  1.9734199373505095  3.8385033657559648  8.0308754104330902   F   F   F
  5.3941958850873633  0.2457085293049778 23.9845127663549498   T   T   T
  4.2842854503561041  0.5384473809384985 28.6506071602743759   T   T   T
  5.8379790127227817 -1.3622255169374033 29.8753849313627633   T   T   T
  6.0653902207614463  0.1033459385071988 33.5919368295368841   T   T   T
  3.6009983499615199  0.1926158543328654 25.9134920005203355   T   T   T
  1.1016763121992383  0.5686605296193732 26.5670074240409839   T   T   T
  3.3139799089534936 -1.1026720105968888 30.5686525733503096   T   T   T
  3.5702248796348002 -0.7034698659290919 33.1161968336956036   T   T   T
  4.6187193500552377  2.5119907867236617 25.2583177974194193   T   T   T
  2.7545347197430643  2.4387202401710035 27.2488800002612628   T   T   T
  4.9552943001397711  0.7849022569871607 31.3068071407089867   T   T   T
  4.1436708869464409  1.9048803677949253 33.5962912300892427   T   T   T
  2.1439211277599641  2.0935296511126369 24.6826036060606846   T   T   T
  0.2357023596024085  2.9189516494477448 27.9208825828209406   T   T   T
  1.7720764662757871  0.9980234180077955 29.2496534183162922   T   T   T
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  2.4259213276740739  1.3933289855280040 31.8157256556372445   T   T   T

Metal reference with oxide lattice constant: O-a-SiO2(0001)/fcc(111)_2x2/Ir
E_tot= -138.60761387 eV
 D3-zero damping= -8.4659468 eV, D3-BJ damping= -8.5447364 eV
Ir
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999983    4.2975558034858610    0.0000000000000000
     0.0000000000000014    0.0000000000000024   22.6258653885799461
  16
Cartesian
  6.6645971591174238 -0.7296945035300652  6.3431065727710330
  4.7998341893538718  0.5955362382472438  9.6714309777277929
  5.1975750155243645 -1.1897074473222102 13.9164815408962035
  6.1318170238574154 -1.3169729346118957 16.3356046968561088
  3.5245471591083470 -1.0659623183361582  8.0874953426880758
  2.2532218908949595  0.0130285242960447 10.3183147370603017
  2.3103684793970554 -1.5278524487910714 12.4445893050672201
  3.6211811145547248 -0.8995941977199201 15.9984524659283611
  4.8788239841151713  1.0371110431721275  7.0607477339784541
  3.5035151595688423  2.6463809040743391  8.7193808117770466
  4.1307910196944357  0.3026652396680813 12.1542741795789055
  4.5612652148916890  1.2480428256050631 14.6419761814194871
  2.3795291294232546  1.6979197428361466  6.5219398376328170
  1.6253861758049113  2.4596389756665169 10.5314631203511961
  1.6727352285842376  0.9578646787523551 12.8508513190849296
  2.0580332141351825  1.0149566640175953 15.4731637821987515

Interface with oxide lattice constant: O-a-SiO2(0001)/fcc(111)_2x2/Rh
E_tot= -328.04108279 eV
 D3-zero damping= -10.0899494 eV, D3-BJ damping= -12.149989 eV
Si  O Si  O Si  O  H Rh
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999983    4.2975558034858610    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.5895319265098493
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.5589578055641864  0.1835607425578427  9.0169746245084799   F   F   F
 -1.2460063245427060  2.3706020739380591 10.8612336967246339   F   F   F
  2.2954873726859057  2.6196387297796453 11.6081185941916640   F   F   F
  3.4828408076011028  1.4113732975935680  9.5654178022134690   F   F   F
 -0.6270092618390269  3.7596400629834137 10.2987723773365882   F   F   F
  1.1042088912653407  3.4333422918536529  8.2518078419286862   F   F   F
 -0.1950063026963110  1.7174372615560010 11.9218080039603844   F   F   F
  2.6069757309659334 -0.0448243720647176 14.5050718430130079   F   F   F
  1.2211146816757126  2.0103212146560763 12.6701466762358930   F   F   F
 -1.3518836137004131  2.2409362614904325 16.3172330782069537   T   T   T
  2.1423395649451873  2.4609535577405706 16.9670704828941332   T   T   T
  3.5636178443333284  1.0883123965860373 15.1677299703568895   T   T   T
  1.7363447519784172  0.6009253703169685 13.2917821082657586   F   F   F
 -0.8650249925097481  3.6422505520288042 15.6450910159477452   T   T   T
  1.0572083999651558  3.0745478039444141 13.8903255655927023   F   F   F
 -0.3422384958379741  1.7768546569285464 17.4998736467876483   T   T   T
 -0.1348451872668059  4.1142727492870996 20.0203707212081099   T   T   T
  1.1111485740072127  2.0792843985332587 18.1618946971094957   T   T   T
  3.7983806314496449  1.9188342044002926 21.8222948564126220   T   T   T
  3.0437772948760520  0.6107241410094547 21.2406833126483932   T   T   T
  1.5475872788569176  0.7577869994259856 18.9795015463872758   T   T   T
 -1.1932392869057773  3.0617525234239320 20.6722633067383121   T   T   T
  1.0208317674463361  3.3316838633583039 19.1885891479925483   T   T   T
```

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  0.3470385071796261  1.5348754638604438 22.3010928526148682   T   T   T
  2.9401460928882663  2.3905828191864860 23.1823301599421221   T   T   T
  1.3773667780178473  0.6802549719477082  7.9999999999999982   F   F   F
  1.1764967236772890  1.6519932737523471  8.0158744918591029   F   F   F
  1.9734199373505095  3.8385033657559648  8.0308754104330848   F   F   F
  6.2809153839419851 -1.2535332972439055 24.9606977797460594   T   T   T
  5.5100448140125131  0.5919263815026304 26.7996690694992701   T   T   T
  5.5907182672508595 -1.4273414451606865 30.3617437843418507   T   T   T
  6.8306304266154925 -1.4293196319838977 32.7524610798349727   T   T   T
  3.8369443890275954 -1.3490649981926652 25.6771912414197558   T   T   T
  3.0372769492438483  0.8111516883621165 27.0541779111879102   T   T   T
  3.1044293442460185 -1.4305603676949823 30.3655975235255227   T   T   T
  4.3466996364684807 -1.4310801432513693 32.7450231928309634   T   T   T
  5.3681012325297903  1.1064857741130489 24.2125654989819417   T   T   T
  4.3660891996231914  2.8711699977687299 27.6810874187562241   T   T   T
  4.3476877773050511  0.7899503035400209 29.4598429645332303   T   T   T
  5.5886445100915587  0.7166234771647303 31.9569541023614860   T   T   T
  2.8767195240773034  0.6755938843583447 24.4522573653679522   T   T   T
  1.8677993746025587  2.8804124854157025 28.1138822782505251   T   T   T
  1.8526359395520415  0.6629768654511985 29.4702710516797417   T   T   T
  3.1080788377739625  0.7218608398025289 31.9378828142688285   T   T   T

Metal reference with oxide lattice constant: O-a-SiO2(0001)/fcc(111)_2x2/Rh
E_tot= -114.59511978 eV
 D3-zero damping= -7.1021531 eV, D3-BJ damping= -8.0874452 eV
Rh
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999983    4.2975558034858610    0.0000000000000000
     0.0000000000000014    0.0000000000000024   22.5577498125709219
  16
Cartesian
  7.4417820320646157 -0.3607413623116101  7.4278409227006899
  5.5175274819306397 -0.0309858155416193  9.2926536869945924
  4.8899451035436199 -1.8094925399279536 12.5776596883136467
  5.4795852982490096 -1.4895438455716878 15.1696022533427044
  4.9286425438546875 -0.3766626969512024  6.8534958588597785
  3.0706257787640374 -0.0400547622675621 10.0165575535789753
  2.4442879493952909 -1.8192750827424613 13.3043199910303116
  3.0295651512127106 -1.4736280169918352 15.7448766602874066
  6.1923106439274207  1.7947160254695902  7.4295614579134970
  4.3019870225242123  2.1250907005977848 10.7683773087626324
  3.6661346412197364  0.2998406129920989 12.5743970808448644
  4.2468863393530381  0.6515615722431762 15.1668275226182310
  3.7237294950673250  1.7998463029252432  8.1498092377856377
  1.8122769873299787  2.1483874809167318 10.0208470305399775
  1.1763776171848614  0.3217112806084795 11.8268030115282521
  1.7531454880142510  0.6472844198396492 14.4440692040685139

Interface with oxide lattice constant: O-a-SiO2(0001)/fcc(111)_2x2/Os
E_tot= -386.63684925 eV
 D3-zero damping= -10.2775114 eV, D3-BJ damping= -12.1068344 eV
Si  O Si  O Si  O  H Os
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999983    4.2975558034858610    0.0000000000000000
     0.0000000000000024    0.0000000000000041   38.6201925396729493
   2   5   3   6   3   7   2  16
Selective dynamics
Cartesian
  2.5589578055641864  0.1835607425578427  9.0169746245084816   F   F   F
 -1.2460063245427060  2.3706020739380591 10.8612336967246357   F   F   F
  2.2954873726859057  2.6196387297796448 11.6081185941916658   F   F   F
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  3.4828408076011028  1.4113732975935676  9.5654178022134708   F   F   F
 -0.6270092618390269  3.7596400629834137 10.2987723773365900   F   F   F
  1.1042088912653407  3.4333422918536529  8.2518078419286880   F   F   F
 -0.1950063026963110  1.7174372615560010 11.9218080039603862   F   F   F
  2.6069757309659334 -0.0448243720647176 14.5050718430130097   F   F   F
  1.2211146816757128  2.0103212146560758 12.6701466762358947   F   F   F
 -1.3533786611696659  2.2457467159078188 16.3168215716426417   T   T   T
  2.1364064416177433  2.4569623232732076 16.9564895391890254   T   T   T
  3.5689342265606974  1.0781794223164585 15.1819636142148742   T   T   T
  1.7363447519784172  0.6009253703169684 13.2917821082657603   F   F   F
 -0.8753979041288702  3.6437731732382002 15.6353210915265723   T   T   T
  1.0572083999651556  3.0745478039444141 13.8903255655927040   F   F   F
 -0.3479203731002437  1.8221090220875096 17.5183172061878167   T   T   T
 -0.1281649768283293  4.1422869092767982 20.0046222934080262   T   T   T
  1.1107474469312044  2.1260559641452987 18.1673926070197140   T   T   T
  3.7902042679848829  1.9193186227383650 21.7996758830246975   T   T   T
  2.9616761818991453  0.6298670363890827 21.2818349400461955   T   T   T
  1.5196407186274026  0.8134018895862271 19.0176346715879134   T   T   T
 -1.1128108141855437  2.9791292759958825 20.5763779760477590   T   T   T
  1.0564582450595930  3.4260596119094773 19.1473724112441843   T   T   T
  0.3241424201666138  1.3651721494292222 22.2459129005544547   T   T   T
  3.1377987046800420  2.6513825755921827 23.1325928050980210   T   T   T
  1.3773667780178473  0.6802549719477081  8.0000000000000000   F   F   F
  1.1764967236772890  1.6519932737523471  8.0158744918591083   F   F   F
  1.9734199373505095  3.8385033657559644  8.0308754104330902   F   F   F
  7.0467334974886517 -0.9338607099103861 24.9542602460856671   T   T   T
  4.9985970327049865  0.3542855188479166 28.1563466849655128   T   T   T
  4.3755166846030411 -0.7401195103654081 30.5342916752587676   T   T   T
  4.9939928568643319  0.3350675882775480 33.0036642905800761   T   T   T
  4.5077617666975778 -0.4653424993405103 25.7123267895217751   T   T   T
  2.5313265177475976  0.3081443388926802 27.2688943348150374   T   T   T
  1.8905912941527458 -0.7421463195028043 29.7597228135496366   T   T   T
  2.5206045220984730  0.3245883203696295 32.2421860163394456   T   T   T
  5.5026003846564455  1.1585273971731795 24.1338922410412380   T   T   T
  3.7132834359680071  2.4943435744359861 27.2771764775519650   T   T   T
  3.1329762180803660  1.4022778300895669 29.7511406636679894   T   T   T
  3.7418489766960814  2.4838685345243299 32.2191258715785338   T   T   T
  2.8782095056295312  1.4854207677864322 24.8959384177500880   T   T   T
  1.2671658168302051  2.4692021974429648 28.1663948189331848   T   T   T
  0.6489451253100836  1.4108992184021820 30.6342821458389487   T   T   T
  1.2681329236682102  2.4783985955108516 33.0071323063124993   T   T   T

Metal reference with oxide lattice constant: O-a-SiO2(0001)/fcc(111)_2x2/Os
E_tot= -173.01748138 eV
 D3-zero damping= -6.9799982 eV, D3-BJ damping= -7.8033624 eV
Os
 1.0000000000000000
     4.9623900000000001    0.0000000000000000    0.0000000000000000
    -2.4811949999999983    4.2975558034858610    0.0000000000000000
     0.0000000000000014    0.0000000000000024   22.5900585277533068
  16
Cartesian
  5.1230301711239132 -0.5584406540643293  7.2660245237933143
  4.8728599876198269 -0.4039186374997458  9.8012872278807137
  5.8933591141518136 -2.0237144586860030 11.6641089850996185
  6.7642084501836743 -0.5805707556214700 15.8202930115807394
  2.6532562011019807 -0.8496026508951439  8.1682130631630052
  2.4279294944245802 -0.0203020338441563 10.8836784478602695
  3.3913677331276499 -1.5861221614613557 12.7539176281741575
  4.3803829151439029 -0.6815017159065386 14.9890722741903133
  4.0714427180748984  1.6563468431229424  6.5587941898085189
  3.3326548231974442  1.6065168340317479  9.0657889693975378
  5.0844003078544162  0.3229784639020177 12.4515643312559714
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  5.3270022717966423  1.6145735466734097 14.9773451398898292
  1.6094576401182088  1.4249960085191868  7.1384440908946072
  0.8251203408010459  1.9066581295159615 10.2553212522802131
  2.5006439965559757  0.6766455035812190 13.5114310280566503
  2.9975981947601626  1.5856312678066409 15.8911740568923410

Interface with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Au E_tot= -
113.44150084 eV
 D3-zero damping= -9.2508661 eV, D3-BJ damping= -9.0165031 eV
Zn  O Zn  O Zn  O Zn  O Au
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.9445817414883919
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.7806608893203433  0.0049405271568292  8.0000000000000000   F   F   F
  1.8904006260623938  2.6463184375445006  8.0000055199296671   F   F   F
  3.7806607808966195  2.0077894291542111  8.0000008619369254   F   F   F
  1.8904013448528427  4.6491673426539926  8.0000049280612373   F   F   F
  0.9452663827325467  0.0049405464826632  9.6370125635575068   F   F   F
  4.7257842589986510  2.6463184568703344  9.6370180834871757   F   F   F
  0.9452662743088222  2.0077894484800445  9.6370134254944340   F   F   F
  4.7257849777890986  4.6491673619798268  9.6370174916187459   F   F   F
  3.7894384083805921  0.0263582391853878 11.3043895696556707   T   T   T
  1.8812539047585828  2.6678747427615792 11.3043753585104199   T   T   T
  3.7468497846386200  2.0093177148311838 11.2861872597862636   T   T   T
  1.9239405009942376  4.6506715253573763 11.2862299269566186   T   T   T
  0.9801992268688802  0.0243812323205441 12.8582058565051440   T   T   T
  4.6905289699459729  2.6660575247917673 12.8581051465047533   T   T   T
  0.8651474224132428  1.9772566454799037 12.8189726509462147   T   T   T
  4.8060079139580871  4.6189018314576122 12.8188051072789460   T   T   T
 -0.8100381556608645 -0.1031222277147043 15.1079589139649038   T   T   T
  2.1762088559812223  1.4620054556413380 17.5514162498456230   T   T   T
  0.7239628800080090  0.3588793220060771 19.8744737491036645   T   T   T
  0.8091452874147763  2.5384749441886769 15.1075203528248903   T   T   T
  0.6408740458137379  3.9886156662676457 17.4747029271014185   T   T   T
 -0.7221423872764926  3.0006442191183753 19.8740220712706588   T   T   T
  2.0959424478128152 -0.1917066894787127 15.1980695163321755   T   T   T
  5.0308800756856353  1.3475405969361671 17.4741305668879470   T   T   T
  3.5558865753238336  0.4299538639949615 19.9180425290072627   T   T   T
  3.5742054645896886  2.4496134319538028 15.1972499656005269   T   T   T
  3.4956138791624203  4.1028230669452972 17.5507055414233442   T   T   T
  2.1170963792200843  3.0720039266044417 19.9197011247559068   T   T   T

Metal reference with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Au
E_tot= -41.0172856 eV
 D3-zero damping= -5.1440345 eV, D3-BJ damping= -5.2332311 eV
Au
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.3282195297109460
  12
Cartesian
 -0.7161092424353999 -1.0829627549114673  7.8741242047382469
  2.1393500723835328  0.5822794121373388 10.2342669171036178
  0.7145790879724251 -0.4026954073000438 12.5947917019258551
  0.7160751788279469  1.5594493867888752  7.8735545127046587
  0.6963680298897329  3.2211435664998804 10.2351669598110906
 -0.7147023431523013  2.2388092427333603 12.5964244198312993
  2.1192957875376446 -1.0799815250031370  7.8752878806145636
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  4.9744596918130997  0.5815677681051060 10.2354501045572217
  3.5500851900985309 -0.4021365218415464 12.5973476687281920
  3.5520043151380727  1.5597535985049249  7.8752334387765996
  3.5315419077970001  3.2255542194757267 10.2361441606136179
  2.1206328277707569  2.2382417802056618 12.5965547726017331

Interface with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Ag E_tot= -
105.77743583 eV
 D3-zero damping= -7.857636 eV, D3-BJ damping= -8.393875 eV
Zn  O Zn  O Zn  O Zn  O Ag
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.9022940497028848
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.7806608893203433  0.0049405271568292  8.0000000000000000   F   F   F
  1.8904006260623936  2.6463184375445001  8.0000055199296671   F   F   F
  3.7806607808966195  2.0077894291542107  8.0000008619369254   F   F   F
  1.8904013448528425  4.6491673426539926  8.0000049280612373   F   F   F
  0.9452663827325466  0.0049405464826632  9.6370125635575068   F   F   F
  4.7257842589986510  2.6463184568703340  9.6370180834871757   F   F   F
  0.9452662743088222  2.0077894484800445  9.6370134254944340   F   F   F
  4.7257849777890986  4.6491673619798259  9.6370174916187459   F   F   F
  3.7651130318297485  0.0089386268562088 11.2905807004765713   T   T   T
  1.9061937144538528  2.6506387192587804 11.2904620006392307   T   T   T
  3.7812355694998763  1.9992669684636561 11.3008866591910682   T   T   T
  1.8904119174596381  4.6406731424962180 11.3009234360532904   T   T   T
  0.9111497726358574 -0.0036580696684731 12.8818296826521248   T   T   T
  4.7598861407089164  2.6374239240639601 12.8820418526833258   T   T   T
  0.9356790474313547  1.9536051821522107 12.8540104560961748   T   T   T
  4.7356409699927990  4.5958797670948863 12.8537984096506150   T   T   T
  0.6117261786422786 -0.8713444854013840 15.3527074454969075   T   T   T
  2.2326222919106122  0.4702365988716833 17.2028743976241216   T   T   T
  0.7064398201006429 -0.7559171330473414 19.9389795403123706   T   T   T
 -0.6110926607458833  1.7701682032419150 15.3529488073841129   T   T   T
  0.6344806927646343  2.8690942193225677 17.6448843448203938   T   T   T
 -0.7061644895818320  1.8846944597888149 19.9393456136481539   T   T   T
  3.3952649765254104 -0.4734689899908127 14.7519096695416039   T   T   T
  5.0366127822397733  0.2280542452587004 17.6451617235381981   T   T   T
  3.5019941832458765 -0.8301075844557860 19.7452665212882685   T   T   T
  2.2765414609458214  2.1676588137537536 14.7513999312324824   T   T   T
  3.4385298630472394  3.1111182055075064 17.2036619944472733   T   T   T
  2.1692412610350660  1.8110738026270978 19.7454109521725556   T   T   T

Metal reference with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Ag
E_tot= -33.37542708 eV
 D3-zero damping= -3.7070814 eV, D3-BJ damping= -4.7067824 eV
Ag
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.3259314419319956
  12
Cartesian
  0.7177752731072481 -1.2916401760733147  7.8993019030413132
  0.7110036977530979  0.3802630394938725 10.2362555814622649
 -0.7136732640897445 -0.5932296894242841 12.5715286547891072
 -0.7010030746725703  1.3498822210875112  7.9028830954849347
  2.1257476792055554  3.0198137692844380 10.2369815870651593
  0.7048767919278297  2.0503709023554744 12.5725819565049761
  3.5524227623862394 -1.2922172615123066  7.9017568674250267
```

```
  3.5465299081362769  0.3794882831572314 10.2375974037238286
  2.1217719499963015 -0.5905157333246788 12.5707912247776292
  2.1340993044082470  1.3490889143886571  7.9025703673504459
  4.9618060188597175  3.0213603460954177 10.2359809667402626
  3.5403198302828960  2.0511808202960005 12.5743586181406606

Interface with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Cu E_tot= -
114.70259307 eV
 D3-zero damping= -6.7032269 eV, D3-BJ damping= -7.8916722 eV
Zn  O Zn  O Zn  O Zn  O Cu
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.7360040983509961
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.7806608893203433  0.0049405271568292  8.0000000000000000   F   F   F
  1.8904006260623936  2.6463184375445006  8.0000055199296671   F   F   F
  3.7806607808966199  2.0077894291542107  8.0000008619369254   F   F   F
  1.8904013448528427  4.6491673426539926  8.0000049280612373   F   F   F
  0.9452663827325466  0.0049405464826632  9.6370125635575068   F   F   F
  4.7257842589986501  2.6463184568703340  9.6370180834871757   F   F   F
  0.9452662743088222  2.0077894484800445  9.6370134254944340   F   F   F
  4.7257849777890995  4.6491673619798268  9.6370174916187459   F   F   F
  3.8004067277749676  0.0092769429778209 11.2948003900923997   T   T   T
  1.8690792814742372  2.6507992598548711 11.2953088615105290   T   T   T
  3.7610949493771502  1.9993392351694244 11.2860733971577325   T   T   T
  1.9069176580757277  4.6405558524158383 11.2868540974217613   T   T   T
  1.0423348866497919 -0.0230421460479298 12.9282398377764007   T   T   T
  4.6261968757406153  2.6172708244313885 12.9292695008323388   T   T   T
  0.9224465098226005  1.9627865106480713 12.9038723643301108   T   T   T
  4.7361591341707294  4.6055106340574508 12.9129130987063530   T   T   T
 -0.0520141791557675 -0.9341231476105631 14.8907502611559952   T   T   T
  1.6059188077872553  0.3284478864501525 16.2234099693530283   T   T   T
 -0.0478684508927859 -0.9246369536971999 17.6028498597716201   T   T   T
  0.0823251916285062  1.7099606903894771 14.8853111886151019   T   T   T
  1.6031760847742706  3.1108812695713053 16.2364523608805875   T   T   T
  0.0773511219234697  1.7181351292046547 17.6010283895088655   T   T   T
  2.9779663087318196 -0.8961581954432771 14.4391987460453191   T   T   T
  4.0978679659551069  0.4687487293111774 16.2366027260351729   T   T   T
  2.9194503247096604 -0.9220388952883294 17.9154272493798246   T   T   T
  2.7179517206271346  1.7420310767085689 14.4468749045345852   T   T   T
  4.0921201831271210  2.9699197404347033 16.2221712598370829   T   T   T
  2.7804932819235821  1.7186792174823811 17.9159074641930545   T   T   T

Metal reference with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Cu
E_tot= -41.93037574 eV
 D3-zero damping= -2.9563166 eV, D3-BJ damping= -3.8680819 eV
Cu
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.6957451068619847
  12
Cartesian
  0.0067159028286375 -1.0083480959356177  8.3383814444635505
  1.4241399119722804  0.3138276502390652  9.8945106278024255
  0.0060841576824808 -1.0094748051937876 11.4496280451906287
 -0.0001035100754116  1.6331036947813917  8.3384268097559744
  1.4245828134190632  2.9502044512923526  9.8942253605236150
  0.0003976749019369  1.6320727864138378 11.4495637459473514
  2.8369666484431999 -1.0113493285216117  8.3329794386468912
```

```
  4.2529207772526290  0.3090252389045124  9.8939636409733964
  2.8363460056580903 -1.0097330264567161 11.4558641984289231
  2.8400433033483408  1.6299793039200510  8.3330362864452692
  4.2530587201989851  2.9552848764469717  9.8942844942723713
  2.8412791787756109  1.6316451504451468 11.4558001697615293

Interface with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Pt E_tot= -
145.07561535 eV
 D3-zero damping= -10.0981766 eV, D3-BJ damping= -9.997652 eV
Zn  O Zn  O Zn  O Zn  O Pt
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.7447317245277034
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.7806608893203433  0.0049405271568292  8.0000000000000000   F   F   F
  1.8904006260623936  2.6463184375445006  8.0000055199296671   F   F   F
  3.7806607808966195  2.0077894291542107  8.0000008619369254   F   F   F
  1.8904013448528427  4.6491673426539926  8.0000049280612373   F   F   F
  0.9452663827325466  0.0049405464826632  9.6370125635575068   F   F   F
  4.7257842589986510  2.6463184568703340  9.6370180834871757   F   F   F
  0.9452662743088222  2.0077894484800445  9.6370134254944340   F   F   F
  4.7257849777890995  4.6491673619798268  9.6370174916187459   F   F   F
  3.9017138242291347  0.0391268235468587 11.3432960327554913   T   T   T
  1.7725068177890340  2.6811593107369180 11.3422964302755584   T   T   T
  3.6407223717020507  1.9898449324501346 11.2117044467807041   T   T   T
  2.0328530936862665  4.6320053802672811 11.2118637583724308   T   T   T
  1.3250504331912685  0.0111208440898615 12.8700364851770779   T   T   T
  4.3510042407768905  2.6524084996464872 12.8683610269291417   T   T   T
  0.6328269605366524  1.8809181881568648 12.7274231687121802   T   T   T
  5.0432463812061155  4.5224602135157195 12.7273116082308064   T   T   T
 -0.1974252794824723 -0.4977423733787636 14.8128099991244095   T   T   T
  1.3701134553636702  0.6698967081326176 16.8820635385540250   T   T   T
 -0.0282267260621733 -0.6650968043148864 18.9013755234260898   T   T   T
  0.1983385905860420  2.1433326727232505 14.8138191291254024   T   T   T
  1.4104689164461357  3.3242412058118456 16.9200787831874422   T   T   T
  0.0336768410792860  1.9763124921444528 18.9018126943574352   T   T   T
  2.7505256021390934 -0.6161445677713829 14.9322720188332827   T   T   T
  4.2643417592421633  0.6827199621452108 16.9220487601486163   T   T   T
  2.8332282981837733 -0.6758353698893012 18.8590757345132189   T   T   T
  2.9245502844443894  2.0253455851836755 14.9316182801467860   T   T   T
  4.3034113906593019  3.3107028045634768 16.8830819850686993   T   T   T
  2.8390938533076588  1.9657598118012640 18.8589935384261160   T   T   T

Metal reference with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Pt
E_tot= -71.71140302 eV
 D3-zero damping= -5.6596081 eV, D3-BJ damping= -5.8829982 eV
Pt
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.9711654014368882
  12
Cartesian
  0.0002317726565658 -0.7318200144814614  8.0367810357031715
  1.4177559401339419  0.5904459070245573 10.0060049300814615
 -0.0012817174215271 -0.7340945519084884 11.9755383670807536
  0.0000736339799923  1.9096138623984369  8.0366753840572613
  1.4181055351474425  3.2320915715465679 10.0050614964120346
  0.0015180838493961  1.9072789557540961 11.9756247450832749
  2.8369848345729771 -0.7309093511206963  8.0361597284032396
```

```
  4.2528738844359300  0.5906021514291838 10.0051041928744038
  2.8356215981692277 -0.7328241317855723 11.9768202626772773
  2.8341912416158692  1.9104756784330226  8.0361953304636771
  4.2531175217939836  3.2317270194397105 10.0061326989452564
  2.8353858161217715  1.9085092991259271 11.9767376217296029

Interface with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Pd E_tot= -
133.92406655 eV
 D3-zero damping= -8.3348134 eV, D3-BJ damping= -9.0166514 eV
Zn  O Zn  O Zn  O Zn  O Pd
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.7989486337601903
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.7806608893203428  0.0049405271568292  8.0000000000000000   F   F   F
  1.8904006260623936  2.6463184375445001  8.0000055199296671   F   F   F
  3.7806607808966195  2.0077894291542102  8.0000008619369254   F   F   F
  1.8904013448528425  4.6491673426539926  8.0000049280612373   F   F   F
  0.9452663827325466  0.0049405464826632  9.6370125635575068   F   F   F
  4.7257842589986510  2.6463184568703335  9.6370180834871757   F   F   F
  0.9452662743088220  2.0077894484800445  9.6370134254944340   F   F   F
  4.7257849777890986  4.6491673619798268  9.6370174916187459   F   F   F
  3.8199736558649806  0.0104748484782585 11.3250631329224269   T   T   T
  1.8507265673483133  2.6517613102844462 11.3250309249043042   T   T   T
  3.7239436794421765  1.9855493486773419 11.2504596920125675   T   T   T
  1.9465988021334948  4.6268760606302211 11.2505771735469704   T   T   T
  1.0957047187818405 -0.0003104921217244 12.8639352918741743   T   T   T
  4.5748011165008675  2.6411169797623097 12.8638444612423886   T   T   T
  0.8504996667147628  1.9492789024192632 12.8608768601582337   T   T   T
  4.8191547313092435  4.5907966910395643 12.8618536839803461   T   T   T
 -0.0015884284896928 -0.7925356857121603 14.9595218971802453   T   T   T
  1.4665901714874290  0.5468912879156073 16.8480316545089330   T   T   T
 -0.0107418035830128 -0.7728761303435719 18.7776396355851922   T   T   T
  0.0036855491215964  1.8489668284878316 14.9588513742815277   T   T   T
  1.4557389480320109  3.1944933392938464 16.8413097744796083   T   T   T
  0.0120140659893277  1.8685887478457457 18.7777897252087058   T   T   T
  2.8098913902917158 -0.7564075017615599 14.7613601219094743   T   T   T
  4.2164793657687882  0.5530636235234648 16.8412147919788282   T   T   T
  2.8592700950357162 -0.7686917506702772 18.8403990067420679   T   T   T
  2.8626767867077567  1.8849155450324331 14.7624194647798905   T   T   T
  4.2054764883785420  3.1881610025381195 16.8482062404817050   T   T   T
  2.8128912001108053  1.8726039508441248 18.8404959070047653   T   T   T

Metal reference with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Pd
E_tot= -60.71588279 eV
 D3-zero damping= -4.1238739 eV, D3-BJ damping= -5.0163385 eV
Pd
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.0463969707155911
  12
Cartesian
 -0.0011896729463286 -0.7759932166259349  8.1037271628540601
  1.4183475620112933  0.5437310557666757 10.0653912020347267
 -0.0000746106076103 -0.7773771347463420 12.0274034616926322
  0.0022922792563966  1.8653797516117048  8.1037267887397935
  1.4184620417598683  3.1855222188552514 10.0643647012332540
  0.0010627885035085  1.8639708397009855 12.0273781296356113
  2.8346763768722365 -0.7769566594555261  8.1024208754688178
```

```
  4.2531371064254326  0.5442430015009558 10.0645332218010140
  2.8356057770315433 -0.7784976830846612 12.0283240762645107
  2.8371960289895788  1.8644098556905171  8.1025249724015502
  4.2533117292849463  3.1851728471094463 10.0654110765954030
  2.8359322301751786  1.8628937181485252 12.0282833143321533

Interface with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Ni E_tot= -
131.51750471 eV
 D3-zero damping= -5.9405352 eV, D3-BJ damping= -6.9944916 eV
Zn  O Zn  O Zn  O Zn  O Ni
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.7024478156635503
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.7806608893203428  0.0049405271568292  8.0000000000000000   F   F   F
  1.8904006260623933  2.6463184375445001  8.0000055199296671   F   F   F
  3.7806607808966195  2.0077894291542107  8.0000008619369254   F   F   F
  1.8904013448528423  4.6491673426539926  8.0000049280612373   F   F   F
  0.9452663827325465  0.0049405464826632  9.6370125635575068   F   F   F
  4.7257842589986501  2.6463184568703340  9.6370180834871757   F   F   F
  0.9452662743088220  2.0077894484800445  9.6370134254944340   F   F   F
  4.7257849777890986  4.6491673619798259  9.6370174916187459   F   F   F
  3.8004524168168277  0.0031630453811289 11.2934986177817613   T   T   T
  1.8706951380822552  2.6445554123504729 11.2935208749405600   T   T   T
  3.7737164815646893  1.9885633786896921 11.2661785488241346   T   T   T
  1.8974385620174943  4.6299529064217699 11.2661468465492174   T   T   T
  1.1743057675604458 -0.0600652804600723 12.9833223250692900   T   T   T
  4.4973536148749913  2.5810072119418317 12.9833787760676742   T   T   T
  0.9909064448932965  1.9530747882437998 12.9783023318695090   T   T   T
  4.6803843334837696  4.5943143936893218 12.9781346634730053   T   T   T
 -0.1374617983146372 -0.7971542473844965 14.7911355612925970   T   T   T
  1.6324013640706898  0.3966396391516018 15.9818914788717983   T   T   T
 -0.0482413926844505 -0.8079354675227851 17.2006433955102516   T   T   T
  0.1380783345224065  1.8441248464993361 14.7911703726548129   T   T   T
  1.6300405779198863  3.2811007051309042 16.0021803127067912   T   T   T
  0.0491230579400768  1.8333040595662777 17.2010382266898567   T   T   T
  3.1048789175847498 -0.7653987345596240 14.2929003839804150   T   T   T
  4.0417224464764319  0.6399594498064000 16.0018812996772688   T   T   T
  2.9765497703137647 -0.8114210377083042 17.8122050730521231   T   T   T
  2.5669774073289804  1.8758963585760040 14.2933037942493950   T   T   T
  4.0392610283930832  3.0381709846831173 15.9820759244870167   T   T   T
  2.6952384881636755  1.8296445027299013 17.8121793403597657   T   T   T

Metal reference with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Ni
E_tot= -57.04555346 eV
 D3-zero damping= -2.498568 eV, D3-BJ damping= -3.3387449 eV
Ni
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.5474811562291535
  12
Cartesian
 -0.0001754249706510 -0.8562222205611314  8.1480315545266109
  1.4465629085122600  0.4531952627894131  9.8121285886339109
  0.0026677911191539 -0.8571034626090891 11.4770000676032264
  0.0003318057652029  1.7852600033287545  8.1480926269340621
  1.4478442929894129  3.0957915659612758  9.8129750722668803
 -0.0017338104304416  1.7842919263739976 11.4768700358342368
  2.8359847875991346 -0.8757712444668234  8.1018429092437714
```

```
  4.2236999916114346  0.4544599651733003  9.8131099570638032
  2.8379687320044353 -0.8563080103468567 11.5235730417356983
  2.8350835036425535  1.7658955227858670  8.1018955085471660
  4.2245545814911267  3.0948006310377925  9.8120308612048781
  2.8330033256721991  1.7845590873140669 11.5235475619296199

Interface with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Ir E_tot= -
173.80603415 eV
 D3-zero damping= -9.2918167 eV, D3-BJ damping= -9.5214956 eV
Zn  O Zn  O Zn  O Zn  O Ir
 1.0000000000000000
     5.6707781395240522    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.5571595945335837
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.7806608893203424  0.0049405271568292  8.0000000000000000   F   F   F
  1.8904006260623936  2.6463184375445001  8.0000055199296671   F   F   F
  3.7806607808966191  2.0077894291542107  8.0000008619369254   F   F   F
  1.8904013448528423  4.6491673426539926  8.0000049280612373   F   F   F
  0.9452663827325465  0.0049405464826632  9.6370125635575068   F   F   F
  4.7257842589986501  2.6463184568703335  9.6370180834871757   F   F   F
  0.9452662743088220  2.0077894484800445  9.6370134254944340   F   F   F
  4.7257849777890986  4.6491673619798259  9.6370174916187459   F   F   F
  3.9449241233443586  0.0549304089323896 11.3499665082477428   T   T   T
  1.7258193659534895  2.6962923909175234 11.3500428437807983   T   T   T
  3.6081158601824117  1.9933277694368874 11.1991902888339023   T   T   T
  2.0626304868346028  4.6347244212992313 11.1993270795868405   T   T   T
  1.4599181945355240  0.0730319516359600 12.8826302824045822   T   T   T
  4.2105519971843384  2.7143925983471964 12.8825958478966136   T   T   T
  0.5067787700072489  1.8234035869534997 12.6675189089770015   T   T   T
  5.1637791043211472  4.4647309329541853 12.6674790661494576   T   T   T
 -0.1094358390376519 -0.8999809128299221 14.7143413029700678   T   T   T
  1.3708428376637072  0.3874024175191705 16.6350433474000354   T   T   T
  0.0012727736905873 -0.9276746565529761 18.4917160132260108   T   T   T
  0.1089541357007160  1.7414066000565547 14.7143477808985352   T   T   T
  1.3654676819641023  3.0482398681410454 16.6244673417293427   T   T   T
 -0.0018507425631233  1.7136720875649110 18.4917256024526395   T   T   T
  2.8265828495080991 -0.9376409786499752 14.8342084475812506   T   T   T
  4.3047521829119395  0.4068890500805439 16.6243823389406238   T   T   T
  2.8336272382680061 -0.9264228718645245 18.4258386887406367   T   T   T
  2.8437080286923853  1.7037527294713770 14.8341800375232928   T   T   T
  4.2994622342385975  3.0288135324425038 16.6350299638860939   T   T   T
  2.8365854617231494  1.7149707095502047 18.4258386803083312   T   T   T

Metal reference with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Ir
E_tot= -99.83635826 eV
 D3-zero damping= -4.9086397 eV, D3-BJ damping= -5.3168646 eV
Ir
 1.0000000000000000
     5.6707781395240522    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7581576368186518
  12
Cartesian
  0.0001395149344409 -0.9454811542903616  8.0628416715614115
  1.4172120324897715  0.3746615340766323  9.8937123324214973
 -0.0003177718047412 -0.9459351281399193 11.7253706098577553
 -0.0005398492372031  1.6958769383562970  8.0628424078236929
  1.4171941675070394  3.0159217093786914  9.8936733541460740
 -0.0000363413763926  1.6954343841944526 11.7253767543123093
  2.8350781167369994 -0.9460358119153864  8.0628104782886574
```

```
  4.2532314471940627  0.3745378435922043  9.8936632261924959
  2.8347079547720289 -0.9458765859483652 11.7249839706322305
  2.8352632538915401  1.6953417764845884  8.0628096228231794
  4.2532152271820554  3.0160320815811876  9.8937142487447129
  2.8357209478167262  1.6954994040279436 11.7249862653755059

Interface with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Rh E_tot= -
155.7184595 eV
 D3-zero damping= -8.1116895 eV, D3-BJ damping= -8.6989305 eV
Zn  O Zn  O Zn  O Zn  O Rh
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.6973210543935302
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.7806608893203428  0.0049405271568292  8.0000000000000000   F   F   F
  1.8904006260623933  2.6463184375445001  8.0000055199296671   F   F   F
  3.7806607808966191  2.0077894291542102  8.0000008619369254   F   F   F
  1.8904013448528423  4.6491673426539917  8.0000049280612373   F   F   F
  0.9452663827325465  0.0049405464826632  9.6370125635575068   F   F   F
  4.7257842589986501  2.6463184568703335  9.6370180834871757   F   F   F
  0.9452662743088220  2.0077894484800445  9.6370134254944340   F   F   F
  4.7257849777890977  4.6491673619798259  9.6370174916187459   F   F   F
  3.8904535101938711  0.0385140797173733 11.3443313876431269   T   T   T
  1.7802390057028006  2.6798829987893167 11.3443668800002726   T   T   T
  3.6549405765543006  1.9969279853104083 11.2244970826750503   T   T   T
  2.0157874291831552  4.6382267232819858 11.2242190856552142   T   T   T
  1.3022890212897178  0.0287842755876617 12.8883390640492603   T   T   T
  4.3682777636731300  2.6697609469279699 12.8888264064633002   T   T   T
  0.6501690838756714  1.9006655309963107 12.7621136960466632   T   T   T
  5.0201059123229133  4.5419131254275493 12.7624516171746265   T   T   T
 -0.1074701390704677 -0.8326699257527488 14.8064903827442151   T   T   T
  1.3981026873983877  0.4680908604584156 16.6537502730674518   T   T   T
 -0.0059495242766979 -0.8449173440940906 18.4391335373522764   T   T   T
  0.1080985824579858  1.8089680462504436 14.8066416651285326   T   T   T
  1.3921913246690669  3.1374540361581835 16.6313093332150110   T   T   T
  0.0053260465623078  1.7958569733621785 18.4389630769624695   T   T   T
  2.8046767217900741 -0.8432181889451725 14.8500505523065716   T   T   T
  4.2785710910200665  0.4959986229910500 16.6299813903202924   T   T   T
  2.8283076770408973 -0.8448018403961494 18.4172268729477118   T   T   T
  2.8660306760324223  1.7985598306526358 14.8506237713172418   T   T   T
  4.2731098551326774  3.1095729054449008 16.6539182814814879   T   T   T
  2.8428471014507672  1.7961601663821516 18.4170226925667748   T   T   T

Metal reference with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Rh
E_tot= -82.0498896 eV
 D3-zero damping= -3.8517236 eV, D3-BJ damping= -4.6729125 eV
Rh
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7288629609639869
  12
Cartesian
  0.0009066742153822 -0.7981945200350686  8.0882225203518647
  1.4185980300095618  0.5240059622395160  9.8788202200937931
  0.0001855776797304 -0.7973156144898432 11.6694582701183958
 -0.0004213090470805  1.8432984558715722  8.0882692613706393
  1.4188420821203485  3.1656019127312938  9.8789053964552664
  0.0001365301685771  1.8440325988047621 11.6694413228421521
  2.8361218035802276 -0.7980006954869587  8.0869424687639562
```

```
  4.2526578236111492  0.5243740372618465  9.8789239464401550
  2.8355503399864421 -0.7976984612570216 11.6710780566924690
  2.8353284369975582  1.8434349987225513  8.0869510941336227
  4.2527895333526144  3.1654828159231623  9.8788246905465069
  2.8356150287753925  1.8436611188866145 11.6710953094273400

Interface with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Os E_tot= -
197.41395754 eV
 D3-zero damping= -7.5288243 eV, D3-BJ damping= -8.5319902 eV
Zn  O Zn  O Zn  O Zn  O Os
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.6509725420282884
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.7806608893203437  0.0049405271568292  8.0000000000000000   F   F   F
  1.8904006260623938  2.6463184375445006  8.0000055199296671   F   F   F
  3.7806607808966199  2.0077894291542107  8.0000008619369254   F   F   F
  1.8904013448528427  4.6491673426539926  8.0000049280612373   F   F   F
  0.9452663827325466  0.0049405464826632  9.6370125635575068   F   F   F
  4.7257842589986510  2.6463184568703340  9.6370180834871757   F   F   F
  0.9452662743088222  2.0077894484800445  9.6370134254944340   F   F   F
  4.7257849777890995  4.6491673619798268  9.6370174916187459   F   F   F
  3.8853178438508897  0.0427144657653690 11.3117994502274115   T   T   T
  1.7855695137432734  2.6841052442743245 11.3119548143388915   T   T   T
  3.6688471497232387  2.0105822355504848 11.2472154392553172   T   T   T
  2.0020128165349096  4.6519722146568787 11.2473124547579300   T   T   T
  1.4205765505819414 -0.0245412503435141 12.9952726965279357   T   T   T
  4.2501413476374683  2.6167709553294762 12.9952604573880048   T   T   T
  0.6354415218970276  1.8860823081264431 12.7236610717014340   T   T   T
  5.0352959170011120  4.5273846104936979 12.7235606813411657   T   T   T
 -0.4372626025933676 -0.7544098657845001 14.7414956649391709   T   T   T
  1.1767357269512666  0.1327562588447903 16.6736869578579920   T   T   T
  0.0529234453349452 -1.1893201026351499 18.6700077782790217   T   T   T
  0.4371156322771537  1.8869246843444145 14.7415651578267060   T   T   T
  1.4372968568230107  2.7402184567033774 16.9612423402685550   T   T   T
 -0.0530048341726572  1.4520608952976652 18.6700327784623354   T   T   T
  2.6376671195423418 -1.3320314342585025 14.9946641059913848   T   T   T
  4.2334178280613184  0.0989986961354074 16.9612051375078607   T   T   T
  2.7857038608590683 -1.1052269345952617 18.6126218112895856   T   T   T
  3.0329495146423988  1.3093426948330877 14.9947575142645100   T   T   T
  4.4939214843399826  2.7741999508795314 16.6737373809560090   T   T   T
  2.8852003966112085  1.5361509629676544 18.6126646551650907   T   T   T

Metal reference with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Os
E_tot= -122.75569347 eV
 D3-zero damping= -3.7888531 eV, D3-BJ damping= -4.5385273 eV
Os
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7545045462142461
  12
Cartesian
 -0.0004479432198031 -0.8829360433156277  8.0461353884232185
  1.5434789684592323  0.4072724564244963  9.8795989680087892
 -0.0020065461127610 -0.8831984859886491 11.7134692542479932
 -0.0007612576710872  1.7015511168645285  8.0460424234810084
  1.2917891813435192  3.0497945122616552  9.8798332332410030
  0.0022355902722651  1.7023287163625602 11.7141104927320470
  2.8370582167964056 -0.9393762121766167  8.0458874995638503
```

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  4.1274016168490277  0.4095617640710167  9.8799234214020064
  2.8356393730321603 -0.9385608003034585 11.7142244084259719
  2.8332650405551267  1.7581439759980795  8.0459033530952606
  4.3781936575783593  3.0497215144283953  9.8799509662902949
  2.8348642600459075  1.7583867655875092 11.7138139961279215

Interface with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Ru E_tot= -
175.99515116 eV
 D3-zero damping= -7.9591774 eV, D3-BJ damping= -8.4875473 eV
Zn  O Zn  O Zn  O Zn  O Ru
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.6808571635188407
   2   2   2   2   2   2   2   2  12
Selective dynamics
Cartesian
  3.7806608893203428  0.0049405271568292  8.0000000000000000   F   F   F
  1.8904006260623936  2.6463184375445006  8.0000055199296671   F   F   F
  3.7806607808966195  2.0077894291542102  8.0000008619369254   F   F   F
  1.8904013448528425  4.6491673426539926  8.0000049280612373   F   F   F
  0.9452663827325466  0.0049405464826632  9.6370125635575068   F   F   F
  4.7257842589986510  2.6463184568703340  9.6370180834871757   F   F   F
  0.9452662743088220  2.0077894484800445  9.6370134254944340   F   F   F
  4.7257849777890986  4.6491673619798268  9.6370174916187459   F   F   F
  3.8273522621572500 -0.0157807463200171 11.3172143023511627   T   T   T
  1.8433983537306093  2.6256124736189319 11.3172529169399585   T   T   T
  3.7553088861138946  1.9729045194101078 11.2358640818267705   T   T   T
  1.9154210243532828  4.6143011526128879 11.2359674137332188   T   T   T
  1.2889815734771741 -0.1134995784539558 12.9707666192709361   T   T   T
  4.3816906996918936  2.5276736372757260 12.9707354321678743   T   T   T
  1.1931509618631293  1.9291530093432805 13.0943247401393457   T   T   T
  4.4772387931088327  4.5703491043231166 13.0944801753763880   T   T   T
 -0.0554297085767124 -0.7676105581703210 14.9489441678943731   T   T   T
  1.5726826912773262  0.4746875615176305 16.5943407661951916   T   T   T
 -0.0269269560598760 -0.7875276001427816 18.2588235960700658   T   T   T
  0.0548604007548766  1.8735971585493547 14.9486421277783332   T   T   T
  1.5652995122090501  3.2558976936772561 16.5614941556446595   T   T   T
  0.0268643444349148  1.8533933599546766 18.2588401604249349   T   T   T
  3.0255084851427938 -0.7710374207704771 14.7149321476040598   T   T   T
  4.1052617739717165  0.6144877201237273 16.5614563054591208   T   T   T
  2.8039480877137692 -0.7876711031266980 18.4376926482049477   T   T   T
  2.6447773910814165  1.8703115913458541 14.7148409629667150   T   T   T
  4.0982495127605763  3.1160438703386228 16.5945017717542953   T   T   T
  2.8664292951963901  1.8535428822361248 18.4376377808998164   T   T   T

Metal reference with oxide lattice constant: ZnO(11-20)/fcc(100)_2x2/Ru
E_tot= -101.32039589 eV
 D3-zero damping= -3.6140989 eV, D3-BJ damping= -4.4372139 eV
Ru
 1.0000000000000000
     5.6707781395240531    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.2827558095945903    0.0000000000000000
     0.0000000000000000    0.0000000000000000   19.7407404535333590
  12
Cartesian
 -0.0009571860596144 -0.7883648785461153  8.1828511911557822
  1.5453168792960101  0.5336106729227484  9.8743864546611739
 -0.0009768618612775 -0.7871572764170277 11.5675980153426821
  0.0008366761920272  1.8530849222776753  8.1830032552518261
  1.5469585363722784  3.1753930417253176  9.8751769673893026
  0.0014966933670067  1.8545138994425014 11.5673897012940632
  2.8355790753820593 -0.7857835371202158  8.0374667601834400
```

```
  4.1239135556890973  0.5333251505567864  9.8754260611449993
  2.8352916937332862 -0.7856564365761061 11.7118795010754067
  2.8350849879434321  1.8556336809910514  8.0377661757810586
  4.1255968600336956  3.1747470819710362  9.8746290977291178
  2.8351647761563337  1.8557458221903838 11.7118335813857612

Interface with oxide lattice constant: ZnO(10-10)/fcc(111)_2sqrt3x2/Au
E_tot= -150.77672399 eV
 D3-zero damping= -11.4591729 eV, D3-BJ damping= -11.0782746 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Au
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876115    4.9110471069564703    0.0000000515656527
    -0.0000005331582847    0.0000001131040208   31.5518368081494067
   2   2   1   1   1   1   3   2   1   2   3   2   1   2  12
Selective dynamics
Cartesian
 -1.8899233270904587  3.2739090161257702  8.0000000461225014   F   F   F
 -1.8686491559575451  3.2723226144000450 13.3183124423827852   T   T   T
 -1.8899227058491606  3.2739096316742211 11.2799069537197152   F   F   F
 -1.8718541278487357  3.2877734620662462 16.4759661204377714   T   T   T
  0.0003322317722852 -0.0001173127562226 10.6413778903952245   F   F   F
  0.0003320725054494 -0.0001182009114443  8.6385289852857206   F   F   F
  0.0195076380972561  0.0158398832373467 15.9302117991442138   T   T   T
  0.0190812817959958 -0.0003146763822873 13.8921161877860264   T   T   T
  0.9454589123733134  1.6368940390100062  7.9999999936571049   F   F   F
  0.9742124312384510  1.6344932005571504 13.3204600324095974   T   T   T
  0.0003375315696642  3.2739126414753033 10.6413779203311822   F   F   F
  0.9454595336146127  1.6368946545584580 11.2799069012543196   F   F   F
  0.0003373723028284  3.2739117533200819  8.6385290152216765   F   F   F
  0.0237121024961108  3.2359749965182583 15.9595346193307090   T   T   T
  1.0088104478485356  1.6182886651129109 16.4755137670333163   T   T   T
  0.0171841423179175  3.2612462233583623 13.9094722737960605   T   T   T
  3.7808411518370870 -0.0001209381057559  7.9999999411917084   F   F   F
  3.7957452598559343 -0.0137017336087563 13.3217024050876205   T   T   T
  2.8357197710334376  1.6368976643595399 10.6413778678657867   F   F   F
  3.7808417730783850 -0.0001203225573049 11.2799068487889222   F   F   F
  2.8357196117666015  1.6368967762043185  8.6385289627562809   F   F   F
  2.9035949366372451  1.6199148061822055 15.9470962310606748   T   T   T
  3.8098274848756515 -0.0354153950609358 16.4766438971325861   T   T   T
  2.8646811978053632  1.6315520312952698 13.9030817351970022   T   T   T
  6.2727766674594365 -1.0072541768593894 18.7308839728790915   T   T   T
  4.1364815726977433  0.2310568087321675 21.3096332828507826   T   T   T
  3.4329023901059506 -1.0020303934016481 23.8692387256743039   T   T   T
  3.4192210657805320 -0.8815587623951063 18.7756949332773289   T   T   T
  1.2855826321769028  0.2197217805043966 21.2303483505412025   T   T   T
  0.5977819381029839 -1.0015989158830494 23.8373782730090937   T   T   T
  4.7958647258436171  1.4994315894570474 18.8272997814735170   T   T   T
  2.7165948115053595  2.6721219286508013 21.2342054030415390   T   T   T
  2.0149869383988950  1.4544359084651994 23.8238962244168313   T   T   T
  1.8861283030774569  1.5276389099241823 18.7398684671109841   T   T   T
 -0.1056178069263417  2.7078711199842171 21.2701108150611233   T   T   T
 -0.8169994095375339  1.4577159370445871 23.8366930174110543   T   T   T

Metal reference with oxide lattice constant: ZnO(10-
10)/fcc(111)_2sqrt3x2/Au E_tot= -41.84222101 eV
 D3-zero damping= -5.4601183 eV, D3-BJ damping= -5.3374929 eV
Au
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876115    4.9110471069564703    0.0000000515656527
    -0.0000003544241829    0.0000000751874280   20.9745103866671023
  12
```

```
Cartesian
  6.5617024391106611 -1.0974242775973262  7.8753749721347122
  4.4282736258208573  0.1232492592084951 10.4847509696738701
  3.7410784362291736 -1.1109287214566450 13.0899314687176123
  3.7255210680487489 -1.0967993284688504  7.8740220136877932
  1.5931182169135543  0.1218145570447742 10.4829147491742365
  0.9049430537733495 -1.1105029309192227 13.0922856501851523
  5.1434792887027658  1.3579166118107577  7.8766985098008728
  3.0090103741585605  2.5781555347394614 10.4839387031178966
  2.3231496024709308  1.3441637406171203 13.0920757201014659
  2.3081466470882366  1.3587852725146228  7.8734710422013725
  0.1747980078382884  2.5783722503241577 10.4828040757386258
 -0.5121500494226391  1.3453535588011707 13.0902180572604045

Interface with oxide lattice constant: ZnO(10-10)/fcc(111)_2sqrt3x2/Ag
E_tot= -143.48638418 eV
 D3-zero damping= -9.7979605 eV, D3-BJ damping= -10.6343094 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Ag
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876115    4.9110471069564703    0.0000000515656527
    -0.0000005293260354    0.0000001122910487   31.3250476784756380
   2   2   1   1   1   1   3   2   1   2   3   2   1   2  12
Selective dynamics
Cartesian
 -1.8899233279270442  3.2739090163032429  8.0000000455235796   F   F   F
 -1.8911288628699803  3.2817700388663344 13.3103544563623437   T   T   T
 -1.8899227070287359  3.2739096319244561 11.2799069531207952   F   F   F
 -1.8909366112355566  3.2932999159532081 16.5337216431954310   T   T   T
  0.0003322306594833 -0.0001173125201532 10.6413778900172655   F   F   F
  0.0003320716020917 -0.0001182007198063  8.6385289849077598   F   F   F
 -0.0032253741412518  0.0256218030762998 15.9421169990949601   T   T   T
  0.0005335181350518  0.0070604462978782 13.9166083008521628   T   T   T
  0.9454589115367286  1.6368940391874789  7.9999999933576440   F   F   F
  0.9481934849389640  1.6403934363740302 13.3096233085190168   T   T   T
  0.0003375304568621  3.2739126417113731 10.6413779199212417   F   F   F
  0.9454595324350378  1.6368946548086925 11.2799069009548596   F   F   F
  0.0003373713994704  3.2739117535117197  8.6385290148117360   F   F   F
 -0.0048854268268601  3.2843671639955372 15.9371419071051061   T   T   T
  0.9493291448870330  1.6556763671475230 16.5299690665595129   T   T   T
  0.0000093702744326  3.2772150809315015 13.9122476161723796   T   T   T
  3.7808411510005020 -0.0001209379282831  7.9999999411917084   F   F   F
  3.7821431678266415  0.0033040103246889 13.3107545491297827   T   T   T
  2.8357197699206362  1.6368976645956095 10.6413778677553061   F   F   F
  3.7808417718988103 -0.0001203223070703 11.2799068487889222   F   F   F
  2.8357196108632441  1.6368967763959568  8.6385289626458004   F   F   F
  2.8434823473190209  1.6542520491752122 15.9391187658969713   T   T   T
  3.7780107703004284  0.0134158122374682 16.5253844180974276   T   T   T
  2.8385019963957556  1.6425518026303023 13.9137398463546837   T   T   T
  6.1766903223087697 -0.8222584717324738 18.7148352200517252   T   T   T
  4.7456868905942553  0.0553218951332079 21.0655252716665409   T   T   T
  4.7215761522232498 -1.5801319186420211 23.4829955818409530   T   T   T
  3.3431955195933605 -0.7079288902267801 18.7132078154913799   T   T   T
  1.8907040082753255  0.0554470860079994 21.0650612551337133   T   T   T
  1.8832455683041074 -1.5797685120001097 23.4789064905706191   T   T   T
  4.7266214937312663  1.6912965331432777 18.6976467881383748   T   T   T
  3.2980539346716120  2.4938673997680527 21.0666363579552147   T   T   T
  3.3048279291690990  0.8720899290807164 23.4800333197666937   T   T   T
  1.8256129349318626  1.6900877955249709 18.7142249723126213   T   T   T
  0.4632699611483239  2.5289753506263222 21.0655009089440490   T   T   T
  0.4704837852553875  0.8780007922683574 23.4778762585118379   T   T   T
```

```
Metal reference with oxide lattice constant: ZnO(10-
10)/fcc(111)_2sqrt3x2/Ag E_tot= -33.63244061 eV
 D3-zero damping= -3.932214 eV, D3-BJ damping= -4.9688796 eV
Ag
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876115    4.9110471069564703    0.0000000515656527
    -0.0000003498994190    0.0000000742275461   20.7067388524177183
  12
Cartesian
  6.1460716734084082 -0.7589342428339009  7.9224285505479202
  4.7271686507083084  0.0578978260821990 10.3481453407730424
  4.7265382199835466 -1.5758972468316674 12.7745441337847367
  3.3105611839278222 -0.7607678319257264  7.9229355663203807
  1.8917727494697383  0.0575502096116455 10.3484422434007737
  1.8907209708398962 -1.5759156776565864 12.7751527274487255
  4.7286052609874334  1.6955956124316918  7.9227541654559976
  3.3102730031199816  2.5129588768088302 10.3483171847293978
  3.3088509449666472  0.8793742998143689 12.7748106180019931
  1.8940032586533340  1.6953779259585959  7.9224917452333052
  0.4741923634817239  2.5126939166144342 10.3483367636440224
  0.4734090053224780  0.8800306272286619 12.7747073886648845

Interface with oxide lattice constant: ZnO(10-10)/fcc(111)_2sqrt3x2/Cu
E_tot= -152.09297627 eV
 D3-zero damping= -8.2358294 eV, D3-BJ damping= -9.5175459 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Cu
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876106    4.9110471069564694    0.0000000515656527
    -0.0000005269489536    0.0000001117867754   31.1843740710124777
   2   2   1   1   1   1   3   2   1   2   3   2   1   2  12
Selective dynamics
Cartesian
 -1.8899233467368735  3.2739090202935532  8.0000000343716913   F   F   F
 -1.8928747104232788  3.2956027594905155 13.2997913045243301   T   T   T
 -1.8899227335503765  3.2739096375507470 11.2799069419689086   F   F   F
 -1.9017705173104618  3.3121659848601523 16.5462667311960949   T   T   T
  0.0003322056391703 -0.0001173072123523 10.6413778831908079   F   F   F
  0.0003320512909345 -0.0001181964110042  8.6385289780813022   F   F   F
 -0.0185481927286729  0.0369161954154804 15.9371471570915997   T   T   T
 -0.0048651451597754  0.0204229341580740 13.9254300885875484   T   T   T
  0.9454588927268993  1.6368940431777901  7.9999999880678621   F   F   F
  0.9452933337988758  1.6537890925229015 13.3004066042742508   T   T   T
  0.0003375054365493  3.2739126470191735 10.6413779124687569   F   F   F
  0.9454595059133972  1.6368946604349843 11.2799068956650768   F   F   F
  0.0003373510883135  3.2739117578205215  8.6385290073592493   F   F   F
 -0.0113158096331950  3.2856827729566054 15.9359438072047901   T   T   T
  0.9530247572199917  1.6609703450980791 16.5433076619887700   T   T   T
 -0.0033853624966302  3.2885863794917691 13.9250383558917310   T   T   T
  3.7808411321906732 -0.0001209339379721  7.9999999417640311   F   F   F
  3.7770380044560077  0.0147073103506166 13.2995848706178510   T   T   T
  2.8357197449003233  1.6368976699034099 10.6413778661649250   F   F   F
  3.7808417453771694 -0.0001203166807782 11.2799068493612467   F   F   F
  2.8357195905520864  1.6368967807047587  8.6385289610554192   F   F   F
  2.8434415680856606  1.6674694253382960 15.9315121608247630   T   T   T
  3.7642610180820335  0.0165641395500316 16.5468169099125006   T   T   T
  2.8377621358409768  1.6556111433775698 13.9214606778803471   T   T   T
  6.3690549824674845 -1.0188229332107162 18.4576516405872368   T   T   T
  4.9606401177156290 -0.1309637454127920 20.3265385603952886   T   T   T
  4.7103129597231579 -1.6113206821472674 22.2847830060713079   T   T   T
  3.3726847383731604 -0.4785561313697941 18.4567717173950179   T   T   T
  1.8773017350503769  0.0276807781534867 20.3825062773720909   T   T   T
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  1.7058060274884193 -1.7222508338433875 22.1524494432160779   T   T   T
  4.7141457432274905  1.6570477459166435 18.6775972772659102   T   T   T
  3.0383578039619556  2.3436290553969097 20.3245972274341753   T   T   T
  3.4762996610045787  0.7511502886799215 22.1527092883186825   T   T   T
  1.5659026109457845  1.5770137963434909 18.4554572253251479   T   T   T
  0.4681394989354870  2.7719684639901789 20.3249472449704349   T   T   T
  0.4512872611309945  1.0464445637338862 22.1519458265393538   T   T   T

Metal reference with oxide lattice constant: ZnO(10-
10)/fcc(111)_2sqrt3x2/Cu E_tot= -41.68431465 eV
 D3-zero damping= -3.0238558 eV, D3-BJ damping= -3.8886204 eV
Cu
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876106    4.9110471069564694    0.0000000515656527
    -0.0000003406878535    0.0000000722734077   20.1616065333788548
  12
Cartesian
  5.8501844950391098 -0.5902383098295507  8.2004938373529139
  4.4388301479522658  0.0408277108509042 10.1470099100023639
  4.4216291605259981 -1.6433286825283839 11.9626059274873171
  3.0290298569495784 -0.5966816224936515  8.2087799809973969
  1.5956794512152426  0.0333233282788935 10.1367529197714585
  1.6111213988954041 -1.6492488905574711 11.9547292600224537
  4.4229071134188906  1.6421640340357431  8.2432740668256557
  3.0077405519735616  2.6414830787326915 10.0269679326430285
  3.0087972633013642  1.0239190056201795 11.9203180913852993
  1.6113291951975437  1.6416981545781624  8.2358214970450963
  0.1820066772889325  2.6184185292163518 10.0156797743767072
  0.1882539303225474  1.0202987080381778 11.9276567239931737

Interface with oxide lattice constant: ZnO(10-10)/fcc(111)_2sqrt3x2/Pt
E_tot= -182.89359972 eV
 D3-zero damping= -11.7025048 eV, D3-BJ damping= -11.8281233 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Pt
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876110    4.9110471069564703    0.0000000515656527
    -0.0000005310410037    0.0000001126548615   31.4265379881648776
   2   2   1   1   1   1   3   2   1   2   3   2   1   2  12
Selective dynamics
Cartesian
 -1.8899233332138603  3.2739090174247867  8.0000000419062012   F   F   F
 -1.9185338011574646  3.2857485070420416 13.3086366952875768   T   T   T
 -1.8899227144830852  3.2739096335058191 11.2799069495034168   F   F   F
 -1.9711744521266521  3.3569257697046111 16.4433476067062614   T   T   T
  0.0003322236271069 -0.0001173110283072 10.6413778877344534   F   F   F
  0.0003320658933021 -0.0001181995087456  8.6385289826249476   F   F   F
 -0.0793994509345884  0.0817511055015968 15.9362420633378559   T   T   T
 -0.0280519537431327  0.0177160859362708 13.9101184681484487   T   T   T
  0.9454589062499121  1.6368940403090224  7.9999999915489557   F   F   F
  0.9464856949348572  1.6363798733826218 13.3064127679255808   T   T   T
  0.0003375234244857  3.2739126432032193 10.6413779174452756   F   F   F
  0.9454595249806881  1.6368946563900557 11.2799068991461713   F   F   F
  0.0003373656906808  3.2739117547227807  8.6385290123357699   F   F   F
 -0.0757759675844075  3.2078513001423299 15.9326430731283910   T   T   T
  0.9965621731629911  1.6461575979497469 16.4638767876451624   T   T   T
 -0.0261928132750982  3.2590909130298717 13.9093735617186773   T   T   T
  3.7808411457136861 -0.0001209368067396  7.9999999411917093   F   F   F
  3.7545552771858643 -0.0121827230968702 13.3039006215616400   T   T   T
  2.8357197628882593  1.6368976660874552 10.6413778670880284   F   F   F
  3.7808417644444607 -0.0001203207257070 11.2799068487889258   F   F   F
  2.8357196051544542  1.6368967776070174  8.6385289619785226   F   F   F
```

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  2.8847462809957505  1.6356180014022736 15.9535286565181149   T   T   T
  3.7070829185158747 -0.0753695290283042 16.4763189557704663   T   T   T
  2.8366461753298036  1.6349997372373697 13.9208651603267395   T   T   T
  6.2928159451297221 -0.8993012635161554 18.5429661436782638   T   T   T
  4.4432402626465359  0.1456977790102207 20.9178924370988710   T   T   T
  4.2605787277223000 -1.4009264305404752 23.0949372821379519   T   T   T
  3.4091921371283758 -0.7309550347406923 18.5570309437742154   T   T   T
  1.5474333293421438  0.1473775943847994 20.8221744556791180   T   T   T
  1.3985101787335299 -1.3985613842089888 23.0692521848272030   T   T   T
  4.6620357769856744  1.6346064180450337 18.7737481581369181   T   T   T
  2.9746860379433642  2.5676541230338081 20.8154171399541177   T   T   T
  2.8081574284579358  1.0493287590838007 23.0901779890890104   T   T   T
  1.7159547091950942  1.6459648476914825 18.5559984509397964   T   T   T
  0.1913881870698876  2.6968921830788792 20.8305650600898637   T   T   T
  0.0060141412858714  1.1050662964980629 23.1094709200543527   T   T   T

Metal reference with oxide lattice constant: ZnO(10-
10)/fcc(111)_2sqrt3x2/Pt E_tot= -73.0486165 eV
 D3-zero damping= -5.5682074 eV, D3-BJ damping= -5.9610758 eV
Pt
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876110    4.9110471069564703    0.0000000515656527
    -0.0000003501420161    0.0000000742790106   20.7210955360654729
  12
Cartesian
  5.8702617570855447 -0.7007246663524199  8.1366344822477394
  4.4325645200934467  0.1298339515589366 10.3702429887082879
  4.4179818201604402 -1.4966928713306906 12.6047115273228414
  3.0339501262893447 -0.7010927264015943  8.1359552411894978
  1.5976322767767066  0.1299647767352726 10.3701560991337054
  1.5829788355879044 -1.4967213015134777 12.6046597683741073
  4.4520270724818820  1.7542525057812841  8.1362546584949591
  3.0148959394461126  2.5856414232750224 10.3699448141978330
  3.0004346049036394  0.9592902025329703 12.6048730566439779
  1.6174231018948273  1.7545742805938436  8.1371519417981819
  0.1791860635476326  2.5855306510189537 10.3693260649113022
  0.1644483865426583  0.9591252717085281 12.6034523248893606

Interface with oxide lattice constant: ZnO(10-10)/fcc(111)_2sqrt3x2/Pd
E_tot= -171.81518028 eV
 D3-zero damping= -10.0406564 eV, D3-BJ damping= -10.8572047 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Pd
 1.0000000000000000
     5.6707697787228737   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876115    4.9110471069564712    0.0000000515656527
    -0.0000005288489827    0.0000001121898469   31.2968161156202989
   2   2   1   1   1   1   3   2   1   2   3   2   1   2  12
Selective dynamics
Cartesian
 -1.8899233343452528  3.2739090176648000  8.0000000411676933   F   F   F
 -1.9019679175284399  3.2803301620445104 13.3126947475027144   T   T   T
 -1.8899227160783354  3.2739096338442346 11.2799069487649088   F   F   F
 -1.9224424981436317  3.3097520635782089 16.4847364392251237   T   T   T
  0.0003322221221603 -0.0001173107090483 10.6413778872684048   F   F   F
  0.0003320646716064 -0.0001181992495755  8.6385289821588991   F   F   F
 -0.0379110613481238  0.0366689335155277 15.9488296760388604   T   T   T
 -0.0127699366972651  0.0065771437491713 13.9156133885690227   T   T   T
  0.9454589051185199  1.6368940405490362  7.9999999911797017   F   F   F
  0.9438590233960561  1.6347349882243694 13.3125560472534037   T   T   T
  0.0003375219195390  3.2739126435224786 10.6413779169397920   F   F   F
  0.9454595233854381  1.6368946567284719 11.2799068987769182   F   F   F
  0.0003373644689851  3.2739117549819508  8.6385290118302862   F   F   F
```

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 -0.0332484771096656  3.2449712628873999 15.9446928985501923   T   T   T
  0.9648938364976732  1.6403695520855937 16.4831711288171370   T   T   T
 -0.0121921828305588  3.2656369856609224 13.9126455413711163   T   T   T
  3.7808411445822938 -0.0001209365667264  7.9999999411917093   F   F   F
  3.7698134453256502 -0.0074982417236856 13.3121944887601735   T   T   T
  2.8357197613833134  1.6368976664067145 10.6413778669518013   F   F   F
  3.7808417628492115 -0.0001203203872912 11.2799068487889258   F   F   F
  2.8357196039327586  1.6368967778661878  8.6385289618422956   F   F   F
  2.8560853039230745  1.6436059540734065 15.9450747013779832   T   T   T
  3.7431856635509555 -0.0252985875836511 16.4841023898845833   T   T   T
  2.8360360892082146  1.6365037927267931 13.9129398119879966   T   T   T
  6.1754955321532234 -0.9095714936859817 18.5411084037810383   T   T   T
  4.7505672823511071 -0.0049519273626767 20.7688687382193606   T   T   T
  4.6967423936247483 -1.6233208108779953 22.9601453893754766   T   T   T
  3.3405097289043493 -0.7076116691476174 18.5399382706600484   T   T   T
  1.8623369853069907  0.0116424446980952 20.7602405550250140   T   T   T
  1.8439285413830184 -1.6216003319971490 22.9759532093496119   T   T   T
  4.7002024287031423  1.6478089747213112 18.6771276069153096   T   T   T
  3.2388891247267053  2.4287212945000745 20.7687529454606867   T   T   T
  3.2864352383145783  0.8166313026360588 22.9768622496777688   T   T   T
  1.7499152276070904  1.6465436066023036 18.5404442209696896   T   T   T
  0.4345243841851382  2.5221906999163517 20.7689098499349569   T   T   T
  0.4521886852444009  0.8472680177513912 22.9767419320982356   T   T   T

Metal reference with oxide lattice constant: ZnO(10-
10)/fcc(111)_2sqrt3x2/Pd E_tot= -61.71202995 eV
 D3-zero damping= -4.0965047 eV, D3-BJ damping= -5.0955421 eV
Pd
 1.0000000000000000
     5.6707697787228737   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876115    4.9110471069564712    0.0000000515656527
    -0.0000003473591737    0.0000000736886593   20.5564093773088672
  12
Cartesian
  6.1086999771990831 -0.8114071165720780  8.0790631523368273
  4.6884551628042610  0.0079944285888971 10.2855079048021487
  4.6812936804047833 -1.6291033666282573 12.4925610425792026
  3.2729431606983326 -0.8113226668914695  8.0790723243648390
  1.8529725116469540  0.0080468328308081 10.2847977423404640
  1.8457987419563040 -1.6289500250240438 12.4919451634598175
  4.6906207209019337  1.6436645465242552  8.0796334036503179
  3.2703555081918654  2.4635512308677399 10.2857023015741227
  3.2637972320686055  0.8262916812737430 12.4920139074969860
  1.8548834572411861  1.6434603047558538  8.0792215115550565
  0.4352637682610752  2.4640165771034175 10.2857147409711782
  0.4282131897318194  0.8267434852293306 12.4920218142330288

Interface with oxide lattice constant: ZnO(10-10)/fcc(111)_2sqrt3x2/Ni
E_tot= -167.84335991 eV
 D3-zero damping= -7.5833769 eV, D3-BJ damping= -8.839939 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Ni
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876110    4.9110471069564703    0.0000000515656527
    -0.0000005267405296    0.0000001117425604   31.1720397232404558
   2   2   1   1   1   1   3   2   1   2   3   2   1   2  12
Selective dynamics
Cartesian
 -1.8899233510638380  3.2739090212114750  8.0000000343716913   F   F   F
 -1.8995346730703404  3.2922677984659932 13.3008773966020435   T   T   T
 -1.8899227396513458  3.2739096388450055 11.2799069419689086   F   F   F
 -1.8685323769499229  3.2361882511953697 16.5562463644504021   T   T   T
  0.0003321998835623 -0.0001173059913596 10.6413778840384374   F   F   F
```

```
  0.0003320466186084 -0.0001181954198185  8.6385289789289317   F   F   F
  0.0036826189010076 -0.0114309737626277 16.0717556520569502   T   T   T
  0.0046376071983854 -0.0042490135106455 13.9939408612482481   T   T   T
  0.9454588883999346  1.6368940440957107  7.9999999892166231   F   F   F
  0.9387244672897344  1.6085189405752967 13.3004099227684875   T   T   T
  0.0003374996809412  3.2739126482401666 10.6413779131937041   F   F   F
  0.9454594998124275  1.6368946617292424 11.2799068968138378   F   F   F
  0.0003373464159874  3.2739117588117073  8.6385290080841983   F   F   F
  0.0043711986971577  3.2640965011037442 15.8769287786131024   T   T   T
  0.9644377259608237  1.6555100920402479 16.5542139862161228   T   T   T
  0.0051586139589209  3.2690831313445528 13.8858957920474371   T   T   T
  3.7808411278637077 -0.0001209330200513  7.9999999440615532   F   F   F
  3.8116553800740980 -0.0041560456973001 13.3000647216764172   T   T   T
  2.8357197391447149  1.6368976711244030 10.6413778680386351   F   F   F
  3.7808417392761999 -0.0001203153865206 11.2799068516587688   F   F   F
  2.8357195858797604  1.6368967816959445  8.6385289629291293   F   F   F
  2.8408921804365410  1.6265233448432781 15.8848065248895924   T   T   T
  3.7513324600084688 -0.0118626317600851 16.5573393729756795   T   T   T
  2.8409855814574421  1.6321442306459149 13.8912489443525384   T   T   T
  5.6732879604677713 -0.0194571865463922 19.4461062463565568   T   T   T
  4.1973941049879535  1.3178723826206222 20.6289415309055890   T   T   T
  4.1666059641257966 -0.6513844113899210 22.2499819250488180   T   T   T
  3.4145557605987951 -0.0281801612904715 18.5002841628060644   T   T   T
  1.9022861426075788  0.5798247971456606 20.6292091599997072   T   T   T
  1.2956801994430533 -1.0127208391342821 22.2485559162986455   T   T   T
  3.9778139927858769  2.9433110174168009 18.4975624833476751   T   T   T
  2.4102465476380384  2.9435284222728213 20.6229531855313120   T   T   T
  2.8351887499750554  1.6135136818274287 22.6646959631648031   T   T   T
  1.1216410182952767  1.9386648238160420 18.4956338696100104   T   T   T
  0.0008197936560143  3.2450818059706572 20.4777568324824770   T   T   T
  0.2076512314402403  1.5917690800465905 22.2498620474887652   T   T   T

Metal reference with oxide lattice constant: ZnO(10-
10)/fcc(111)_2sqrt3x2/Ni E_tot= -57.53637604 eV
 D3-zero damping= -2.6917176 eV, D3-BJ damping= -3.5629387 eV
Ni
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876110    4.9110471069564703    0.0000000515656527
    -0.0000003387580026    0.0000000718640098   20.0473996618865868
  12
Cartesian
  5.8353005285447574 -0.6037572510924134  8.2449993239988437
  4.4254142903042712  0.2248370679700814 10.0302083299639158
  4.4327204282496906 -1.4116779079971429 11.8185693067003701
  3.0010023192440638 -0.6017804514628355  8.2392028494438119
  1.5945917328675612  0.2197321123247839 10.0294705791449772
  1.5936385005835279 -1.4139962216283049 11.8183910232412313
  4.4189309466587368  1.8554009653689902  8.2444492131919631
  3.0066803070929398  2.6764426694156263 10.0323779325427136
  3.0134328210542809  1.0414904055751113 11.8192028525665709
  1.5814125480418604  1.8516425958259357  8.2440431015986295
  0.1744695278718187  2.6853926049919221 10.0293197150074995
  0.1809136431094548  1.0459119130714618 11.8135566026707526

Interface with oxide lattice constant: ZnO(10-10)/fcc(111)_2sqrt3x2/Ir
E_tot= -212.38538611 eV
 D3-zero damping= -10.7908179 eV, D3-BJ damping= -11.2190029 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Ir
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876110    4.9110471069564703    0.0000000515656527
    -0.0000005275409457    0.0000001119123604   31.2194076421567850
```

```
   2   2   1   1   1   1   3   2   1   2   3   2   1   2  12
Selective dynamics
Cartesian
 -1.8899233360363688  3.2739090180235531  8.0000000400859008   F   F   F
 -1.8967810596063346  3.2876566413566048 13.2979324574102140   T   T   T
 -1.8899227184627894  3.2739096343500718 11.2799069476831164   F   F   F
 -1.9370027779828132  3.3662222639091670 16.5043235939227451   T   T   T
  0.0003322198726843 -0.0001173102318452 10.6413778865857171   F   F   F
  0.0003320628455117 -0.0001181988621884  8.6385289814762114   F   F   F
 -0.0468203805808234  0.0748469373636621 15.9395289598242069   T   T   T
 -0.0086852899971484  0.0146308289650855 13.9277091006364593   T   T   T
  0.9454589034274036  1.6368940409077886  7.9999999906388055   F   F   F
  0.9634426338798880  1.6327255364528019 13.2987547665596271   T   T   T
  0.0003375196700633  3.2739126439996808 10.6413779161993425   F   F   F
  0.9454595210009837  1.6368946572343088 11.2799068982360211   F   F   F
  0.0003373626428908  3.2739117553693378  8.6385290110898367   F   F   F
 -0.0398750096066035  3.1916001473956253 15.9331136270540323   T   T   T
  1.0560266018753131  1.6334499047093700 16.5026402884221071   T   T   T
 -0.0081117893378802  3.2537731913523813 13.9232307028760705   T   T   T
  3.7808411428911768 -0.0001209362079736  7.9999999411917102   F   F   F
  3.7746884939199847 -0.0178974766666494 13.2987486692425225   T   T   T
  2.8357197591338363  1.6368976668839175 10.6413778667522472   F   F   F
  3.7808417604647562 -0.0001203198814539 11.2799068487889240   F   F   F
  2.8357196021066637  1.6368967782535748  8.6385289616427414   F   F   F
  2.9291483898292765  1.6407884688220151 15.9308604419084130   T   T   T
  3.7230309989501293 -0.0912211104597566 16.5020718646843001   T   T   T
  2.8576253149889119  1.6353453047522888 13.9215859738501493   T   T   T
  6.2163639607269250 -0.9299896147141986 18.5883962987284903   T   T   T
  4.7887963295934171 -0.0190997642645985 20.7119940889181002   T   T   T
  4.7235522028154557 -1.6252898087387724 22.8366055224708120   T   T   T
  3.3728934340947889 -0.6850075932477017 18.5880670258032197   T   T   T
  1.8881679468368191  0.0094259658151216 20.6877851278072349   T   T   T
  1.8864860935342316 -1.6175658066191589 22.8213432144288184   T   T   T
  4.7229848607389133  1.6460042008786870 18.6945450609152992   T   T   T
  3.2475769692318255  2.4235376076407067 20.7128840540996144   T   T   T
  3.2998908327704797  0.8228406622865739 22.8210636207559254   T   T   T
  1.7470767191822989  1.6402176937548427 18.5882146610041055   T   T   T
  0.4633126863240413  2.5359231662267048 20.7126146168394918   T   T   T
  0.4788895966847536  0.8272890680111560 22.8211207065906336   T   T   T

Metal reference with oxide lattice constant: ZnO(10-
10)/fcc(111)_2sqrt3x2/Ir E_tot= -101.85896388 eV
 D3-zero damping= -4.8623653 eV, D3-BJ damping= -5.3830987 eV
Ir
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876110    4.9110471069564703    0.0000000515656527
    -0.0000003441050652    0.0000000729983338   20.3638341072982421
  12
Cartesian
  6.1414893164257691 -0.8116377251802518  8.0833990964883924
  4.7243983317730134  0.0071860937821475 10.1921988093058218
  4.7244620078422734 -1.6300562447369320 12.3015334764303468
  3.3073525935043326 -0.8119020534352466  8.0833995288657050
  1.8889717816861993  0.0068272110372854 10.1914946227031287
  1.8887320486980630 -1.6295518864709524 12.3013394530567020
  4.7245939050960750  1.6440062922563499  8.0827505383682752
  3.3068342519472247  2.4621265762892368 10.1920841713555976
  3.3063792444184159  0.8250548924609891 12.3013678270545874
  1.8891509628955927  1.6445799147157603  8.0834278446132561
  0.4708499045356283  2.4623433178151486 10.1921955157495976
  0.4719820339522826  0.8254202632303236 12.3013072709395601
```

```
Interface with oxide lattice constant: ZnO(10-10)/fcc(111)_2sqrt3x2/Rh
E_tot= -193.88201281 eV
 D3-zero damping= -9.7573526 eV, D3-BJ damping= -10.4720451 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Rh
 1.0000000000000000
     5.6707697787228737   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876110    4.9110471069564712    0.0000000515656527
    -0.0000005269317633    0.0000001117831286   31.1833567658601716
   2   2   1   1   1   1   3   2   1   2   3   2   1   2  12
Selective dynamics
Cartesian
 -1.8899233380082257  3.2739090184418616  8.0000000388567969   F   F   F
 -1.8991307679677518  3.2795356895235561 13.3000691257407979   T   T   T
 -1.8899227212430845  3.2739096349398831 11.2799069464540125   F   F   F
 -1.9230897689490005  3.3197185057685048 16.4949332808375999   T   T   T
  0.0003322172497754 -0.0001173096754222 10.6413778858100692   F   F   F
  0.0003320607162691 -0.0001181984104916  8.6385289807005634   F   F   F
 -0.0406033457762353  0.0360487560797276 15.9352738490731056   T   T   T
 -0.0110411854063378  0.0061461873827618 13.9194154541685045   T   T   T
  0.9454589014555470  1.6368940413260977  7.9999999900242535   F   F   F
  0.9504021453218549  1.6324644174044896 13.3004314719873360   T   T   T
  0.0003375170471544  3.2739126445561038 10.6413779153580652   F   F   F
  0.9454595182206890  1.6368946578241199 11.2799068976214691   F   F   F
  0.0003373605136482  3.2739117558210342  8.6385290102485595   F   F   F
 -0.0306580313816514  3.2259291404863171 15.9341891128493263   T   T   T
  0.9870619304348314  1.6278258145247988 16.4956040100824026   T   T   T
 -0.0099719937855397  3.2597736772032371 13.9188039735316860   T   T   T
  3.7808411409193208 -0.0001209357896645  7.9999999411917093   F   F   F
  3.7706605745338675 -0.0123677597634871 13.3004483331761012   T   T   T
  2.8357197565109282  1.6368976674403404 10.6413778665255201   F   F   F
  3.7808417576844615 -0.0001203192916430 11.2799068487889240   F   F   F
  2.8357195999774216  1.6368967787052715  8.6385289614160143   F   F   F
  2.8717852516315348  1.6388908139107727 15.9344604854082910   T   T   T
  3.7370184105760429 -0.0461041866964657 16.4960383437121969   T   T   T
  2.8426830625464068  1.6341466256813673 13.9186878562043450   T   T   T
  6.2117569307496030 -0.9547251680522946 18.5495177091952073   T   T   T
  4.7880161379473867 -0.0347739049016002 20.6093478613641743   T   T   T
  4.7131468455168859 -1.6440131278189263 22.6905035878867949   T   T   T
  3.3678664680085109 -0.6905977014664856 18.5493229048119588   T   T   T
  1.8778228108717656 -0.0054729326947997 20.5944990657620650   T   T   T
  1.8714113026069583 -1.6397311268145907 22.6688013531886767   T   T   T
  4.7118519654846471  1.6319450889338649 18.6406651423113345   T   T   T
  3.2291430515847717  2.3996087126814682 20.6102210269594437   T   T   T
  3.2943832275355014  0.8063872733181386 22.6686304194304711   T   T   T
  1.7216527320086543  1.6267526103695944 18.5492054197118499   T   T   T
  0.4466744589135644  2.5299401346060382 20.6105426835240380   T   T   T
  0.4658058309246285  0.8139366606539027 22.6685304831961503   T   T   T

Metal reference with oxide lattice constant: ZnO(10-
10)/fcc(111)_2sqrt3x2/Rh E_tot= -83.06923059 eV
 D3-zero damping= -3.850023 eV, D3-BJ damping= -4.7353 eV
Rh
 1.0000000000000000
     5.6707697787228737   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876110    4.9110471069564712    0.0000000515656527
    -0.0000003431930046    0.0000000728048496   20.3098591647433935
  12
Cartesian
  6.0239517374596474 -0.7059213121124375  8.1066610351451711
  4.6001043017311574  0.1121534474205834 10.1606838904163261
  4.5996570846071574 -1.5262631580949644 12.2157553057848123
  3.1882903750025471 -0.7055726501019993  8.1062919453619813
  1.7646071751369159  0.1126422620488585 10.1607876419763912
```

```
  1.7630006262669529 -1.5253580518373691 12.2147349609110218
  4.6060664692040421  1.7497517407284173  8.1065912252694687
  3.1820506596999913  2.5680653830146540 10.1607595092578702
  3.1819628620034481  0.9286245304656703 12.2150661487800107
  1.7700995961379562  1.7493518490832325  8.1062097979012098
  0.3469745305006171  2.5677845187134687 10.1610268646672779
  0.3462805764087909  0.9306838099009445 12.2151276503318336

Interface with oxide lattice constant: ZnO(10-10)/fcc(111)_2sqrt3x2/Os
E_tot= -237.13573916 eV
 D3-zero damping= -9.1452122 eV, D3-BJ damping= -10.3796443 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Os
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876110    4.9110471069564703    0.0000000515656527
    -0.0000005280940663    0.0000001120296992   31.2521408332383182
   2   2   1   1   1   1   3   2   1   2   3   2   1   2  12
Selective dynamics
Cartesian
 -1.8899233363829386  3.2739090180970734  8.0000000398673947   F   F   F
 -1.8970816370882255  3.2842032053107260 13.2955971836099511   T   T   T
 -1.8899227189514487  3.2739096344537355 11.2799069474646103   F   F   F
 -1.9254331291378954  3.3396364407025416 16.5405574524452739   T   T   T
  0.0003322194116872 -0.0001173101340495 10.6413778864478274   F   F   F
  0.0003320624712804 -0.0001181987827991  8.6385289813383199   F   F   F
 -0.0480671930250830  0.0407886866960120 15.9391608054679654   T   T   T
 -0.0107807207898375  0.0094501442502149 13.9332523125175936   T   T   T
  0.9454589030808340  1.6368940409813098  7.9999999905295525   F   F   F
  0.9542600334857164  1.6319693294572764 13.2959316932208313   T   T   T
  0.0003375192090659  3.2739126440974764 10.6413779160497839   F   F   F
  0.9454595205123247  1.6368946573379728 11.2799068981267681   F   F   F
  0.0003373622686591  3.2739117554487263  8.6385290109402781   F   F   F
 -0.0297675707682290  3.2180012487606047 15.9328008958609963   T   T   T
  1.0079311958866566  1.6235545522184942 16.5392306179464192   T   T   T
 -0.0075044609931158  3.2591549364873447 13.9282654878322258   T   T   T
  3.7808411425446082 -0.0001209361344524  7.9999999411917093   F   F   F
  3.7733058806789175 -0.0110321195597802 13.2952435211284463   T   T   T
  2.8357197586728402  1.6368976669817130 10.6413778667119416   F   F   F
  3.7808417599760977 -0.0001203197777899 11.2799068487889258   F   F   F
  2.8357196017324324  1.6368967783329638  8.6385289616024359   F   F   F
  2.8803966974787456  1.6435794851694905 15.9338351383196315   T   T   T
  3.7203414701719040 -0.0593303014056967 16.5394340909067736   T   T   T
  2.8477449811361359  1.6371909322192797 13.9288861819079415   T   T   T
  6.2653202807339810 -0.9892565831467193 18.6656546622469186   T   T   T
  4.8120738999782846 -0.1392847729204431 20.7494008884195722   T   T   T
  4.7092677806845078 -1.6287076358855708 22.8970877497004324   T   T   T
  3.3752094163581243 -0.6047857452410494 18.6650314227108609   T   T   T
  1.8730013680846909  0.0076348323561769 20.7756016210287875   T   T   T
  1.8521937336492753 -1.7308602823583779 22.8293399856128971   T   T   T
  4.7080686988069180  1.6434928175603816 18.8167416478254843   T   T   T
  3.1118032101500090  2.4453250697871720 20.7501650122173835   T   T   T
  3.3876137958496639  0.8588957830632798 22.8297132133722940   T   T   T
  1.6514754671612426  1.6117591959124473 18.6649790123575805   T   T   T
  0.5301167821039786  2.6252357213417494 20.7500150103944456   T   T   T
  0.3777143447995737  0.8942694745248968 22.8294945609994464   T   T   T

Metal reference with oxide lattice constant: ZnO(10-
10)/fcc(111)_2sqrt3x2/Os E_tot= -126.82030463 eV
 D3-zero damping= -3.8496708 eV, D3-BJ damping= -4.6575145 eV
Os
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876110    4.9110471069564703    0.0000000515656527
```

```
    -0.0000003432739393    0.0000000728220191   20.3146488103989213
  12
Cartesian
  6.2007577421184701 -0.8631765945705893  8.0555980288414553
  4.8146958928172578 -0.0636224455824154 10.1457652136235623
  4.6247962515964423 -1.5899927352567746 12.2585695254157887
  3.2527343659331183 -0.7967702269850288  8.1123864005807391
  1.7572781047944721  0.0636493043983382 10.1687179549823341
  1.9036651216889426 -1.6555892340043923 12.2025983267440044
  4.6686061516967543  1.6555522347974680  8.1125137816623827
  3.1768475836694141  2.5212706566635408 10.1691240464233150
  3.3211712006878145  0.8005964269712568 12.2021079503480312
  1.9488189187461364  1.5920592993508205  8.0562031257872579
  0.5622359504942591  2.3926314504986546 10.1456900881145149
  0.3726937661349357  0.8649464537868751 12.2590479539746973

Interface with oxide lattice constant: ZnO(10-10)/fcc(111)_2sqrt3x2/Ru
E_tot= -215.04470099 eV
 D3-zero damping= -9.5200693 eV, D3-BJ damping= -10.2060838 eV
Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Zn  O Ru
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876110    4.9110471069564712    0.0000000515656527
    -0.0000005267755165    0.0000001117499825   31.1741102178194787
   2   2   1   1   1   1   3   2   1   2   3   2   1   2  12
Selective dynamics
Cartesian
 -1.8899233386239291  3.2739090185724766  8.0000000384799232   F   F   F
 -1.8966560889413011  3.2822034678102696 13.2970069386884635   T   T   T
 -1.8899227221112194  3.2739096351240495 11.2799069460771388   F   F   F
 -1.9127225618630095  3.3198280003924472 16.5226029642251255   T   T   T
  0.0003322164307835 -0.0001173095016816 10.6413778855722363   F   F   F
  0.0003320600514225 -0.0001181982694512  8.6385289804627305   F   F   F
 -0.0433123834321839  0.0306807093628532 15.9388569675109064   T   T   T
 -0.0105208564458044  0.0063038122619060 13.9266997894895255   T   T   T
  0.9454589008398434  1.6368940414567130  7.9999999898358167   F   F   F
  0.9483766447300919  1.6339277438790618 13.2979035972631312   T   T   T
  0.0003375162281625  3.2739126447298452 10.6413779151001080   F   F   F
  0.9454595173525540  1.6368946580082857 11.2799068974330332   F   F   F
  0.0003373598488015  3.2739117559620747  8.6385290099906022   F   F   F
 -0.0234114422302364  3.2399616508053062 15.9336502470914123   T   T   T
  0.9742843345667995  1.6292343540851866 16.5140616631437034   T   T   T
 -0.0072568770257393  3.2647186720406354 13.9229874656867860   T   T   T
  3.7808411403036168 -0.0001209356590494  7.9999999411917093   F   F   F
  3.7717370849995588 -0.0063371131387196 13.2974339906896706   T   T   T
  2.8357197556919358  1.6368976676140812 10.6413778664560006   F   F   F
  3.7808417568163266 -0.0001203191074772 11.2799068487889258   F   F   F
  2.8357195993125743  1.6368967788463120  8.6385289613464948   F   F   F
  2.8586339468728981  1.6537345921662965 15.9319409200601960   T   T   T
  3.7307408471827479 -0.0236844846998800 16.5145726165201339   T   T   T
  2.8406324507137621  1.6393083088478260 13.9218705644874241   T   T   T
  6.2921698626078459 -1.0296195201270650 18.6061351932886723   T   T   T
  4.8621496968298414 -0.1563006704160930 20.6147697117807169   T   T   T
  4.6767955756818482 -1.6073117205549641 22.7118404576005730   T   T   T
  3.3826095980360877 -0.5189912404665402 18.6019813646438443   T   T   T
  1.8518667301269167  0.0250559217171213 20.6716125942760449   T   T   T
  1.8126379793020431 -1.7317675175456859 22.6231252191992205   T   T   T
  4.6877768454936843  1.6604289173650955 18.7406907449422206   T   T   T
  3.0257237323989710  2.4135709835148198 20.6186322848524206   T   T   T
  3.3934181509565917  0.8755957208445487 22.6246517973490562   T   T   T
  1.5595131651117169  1.6175400230430499 18.6043146614073045   T   T   T
  0.4978537584893200  2.7204850485922791 20.6165146913386828   T   T   T
  0.3382621865426366  0.9361824955770079 22.6225768655512240   T   T   T
```

```
Metal reference with oxide lattice constant: ZnO(10-
10)/fcc(111)_2sqrt3x2/Ru E_tot= -103.91780187 eV
 D3-zero damping= -3.6776055 eV, D3-BJ damping= -4.5291942 eV
Ru
 1.0000000000000000
     5.6707697787228728   -0.0000048259170827   -0.0000000882045183
    -2.8353890707876110    4.9110471069564712    0.0000000515656527
    -0.0000003421196359    0.0000000725771455   20.2463381494286416
  12
Cartesian
  5.9927032387581063 -0.6646706507207890  8.1499907228633841
  4.3964218394586823  0.0347663648369803 10.0957242189051559
  4.6408705173469205 -1.4451943804305611 12.1662037500177114
  2.9921890560315831 -0.7661815485068635  8.0816631286909768
  1.8292116378442160  0.2075479926315201 10.1460185835185630
  1.6473639836242211 -1.5365077785232473 12.0897062709099270
  4.5721402148445236  1.7827021112873451  8.1556883440447425
  2.9699045427096351  2.5098932680389536 10.0951452629787148
  3.2296223478283279  1.0158092532644449 12.1589770959924284
  1.5754701878086859  1.7008446921807134  8.0775024977011274
  0.4108204735802209  2.6543455116501562 10.1485274403142878
  0.2289591428325409  0.9173117329365580 12.0911373360053105
```