

Supporting Information

Vanadium Oxide Oligomers and Ordered Monolayers Supported on CeO₂(111): Structure and Stability Studied by Density Functional Theory

Christopher Penschke, Joachim Paier, and Joachim Sauer*

Institut für Chemie, Humboldt-Universität zu Berlin, Unter den Linden 6, 10099 Berlin,
Germany

*E-mail: js@chemie.hu-berlin.de.

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1. Description of supported V_nO_{2n} structures

In what follows we will describe the structures of surface V_nO_{2n} clusters with $n = 4 - 8$. The most stable structure of a given composition will be labeled V_nO_{2n} -a and is shown in Figure 1. V_4O_8 . V_4O_8 -a is a chain shaped like a horseshoe. It can be formed by joining two dimers. The pseudovacancy is located inside the horseshoe. Isomers include an eight-membered (V-O)₄ ring (+0.38 eV relative to V_4O_8 -a), a V_3O_7 chain (created by connecting a VO_3 unit to a V_2O_4 chain) in proximity to a VO monomer (+0.47 eV), and a V_2O_4 ring connected to a V_2O_4 chain (+0.78 eV). Structures formed by connecting a VO_2 unit to oxygen atoms from a V_3O_6 ring, either to a vanadyl oxygen atom (+0.99 eV) or to a bridging (ring) oxygen atom (+1.35 eV), are energetically unfavorable.

V_5O_{10} . V_5O_{10} -a is formed by extending the V_4O_8 -a chain by one VO_2 unit. Other isomers are V_3O_6 in proximity to V_2O_4 (+0.14 eV relative to V_5O_{10} -a), a 10-membered ring created by connecting both ends of a V_4O_8 -a chain with one VO_2 unit (+0.46 eV), a V_3O_6 ring connected to a V_2O_4 chain via a vanadyl oxygen atom of the trimer (+0.48 eV), and a V_4O_9 chain in proximity to a VO monomer (+0.53 eV).

V_6O_{12} . V_6O_{12} -a consists of a 12-membered (V-O)₆ ring. Two adjacent V_3O_6 rings (+0.29 eV relative to V_6O_{12} -a), a chain structure formed by adding one VO_2 unit to both ends of a V_4O_8 -a chain (+0.65 eV), and a V_3O_6 ring next to a V_3O_6 chain (+0.92 eV) are less stable.

V_7O_{14} . V_7O_{14} -a features a 14-membered ring. It may be created from V_6O_{12} -a by connecting one oxygen atom of the additional VO_2 unit to a V atom from the ring, simultaneously breaking one of the bridging V-O bonds. This bridging O atom forms a double bond to its other attached V atom, creating a vanadyl group (parallel to the surface and pointing inside the ring), while the former vanadyl O atom of this V atom binds to the V atom of the additional VO_2 unit. Other isomers may be formed by adding a VO_2 unit to a V_6O_{12} -a ring, either via a vanadyl O atom (+0.21 eV relative to V_7O_{14} -a), by placing the VO_2 unit inside the ring (+0.32 eV), or by insertion into an anchoring V-O bond (+0.74 eV). The latter results in an elevated V=O unit in the ring. Further examples are a distorted 14-membered ring structure, which may also be described as a 10-membered ring attached to a V-O-V bridging oxygen atom of a nearby V_2O_4 ring (+0.45 eV), and an extended (infinite) curved chain structure (+0.60 eV), which contains a bond between an oxygen atom on one end and the periodic image of a vanadium atom from the other end.

V_8O_{16} . V_8O_{16} -a is based on a V_6O_{12} -a ring which is linked with its periodic replica by a V_2O_4 unit, resulting in an infinite $[(VO_2)_6-(VO_2)_2-]$ configuration. In contrast to the V_6O_{12} -a ring,

however, one additional oxygen atom is added between two vanadium atoms, leading to a V_2O_4 ring as part of the V_6O_{12} ring. Alternatively, the structure may be described as a wavy extended chain built from V_6O_{12} repeat units with two vanadyl oxygen atoms coordinated to the V atoms of a V_2O_4 ring. Other isomers are a 16-membered ring created by insertion of a VO_2 unit into a V_7O_{14} ring, which may also be obtained by addition of a V_2O_4 unit to a V_6O_{12} ring (+0.02 eV relative to V_8O_{16} -a), a distorted V_7O_{14} ring connected to its periodic replica by a VO_2 unit (+0.42 eV), a structure similar to V_8O_{16} -a but containing a distorted V_6O_{12} ring (+0.68 eV), and a highly distorted 12-membered ring connected with a V_2O_4 chain in an e-shaped arrangement (+0.70 eV).

2. Structure of a supported V_2O_5 cluster

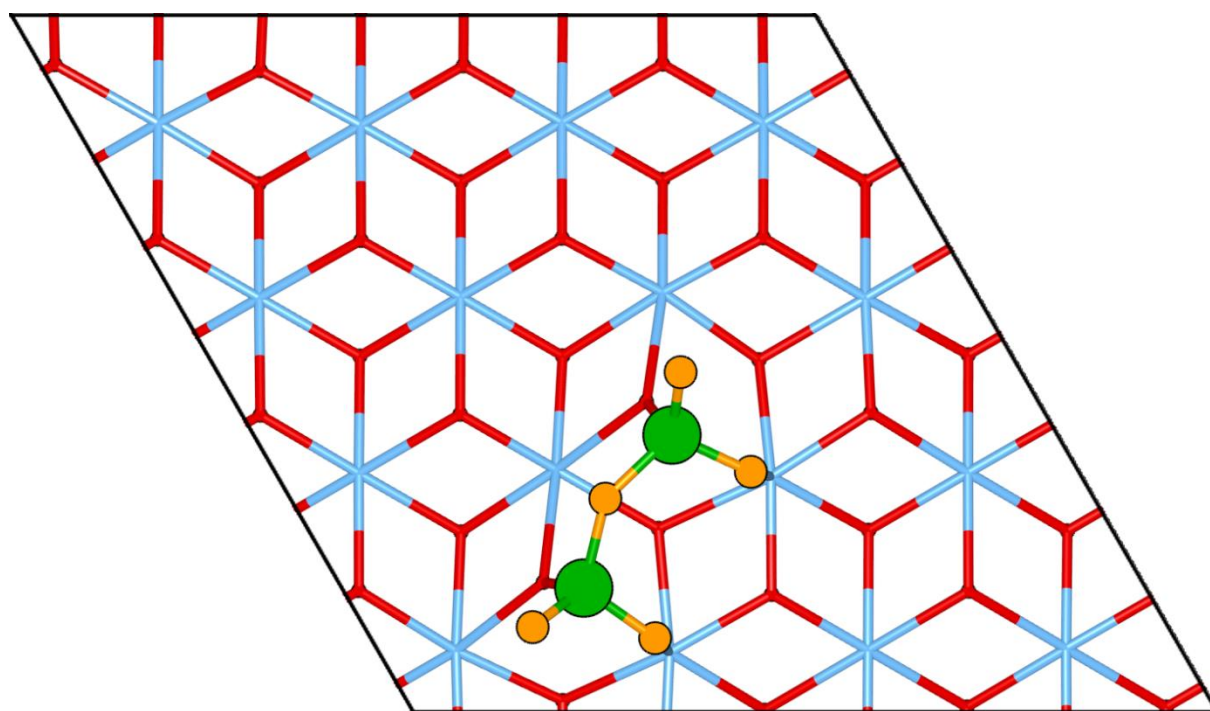


Figure S1 Top view of the V_2O_5 cluster supported on $CeO_2(111)$. For details and color code, see Figure 1. Black lines indicate primitive unit cells.

3. Alternative VO₂ and V₂O₅ monolayer structures

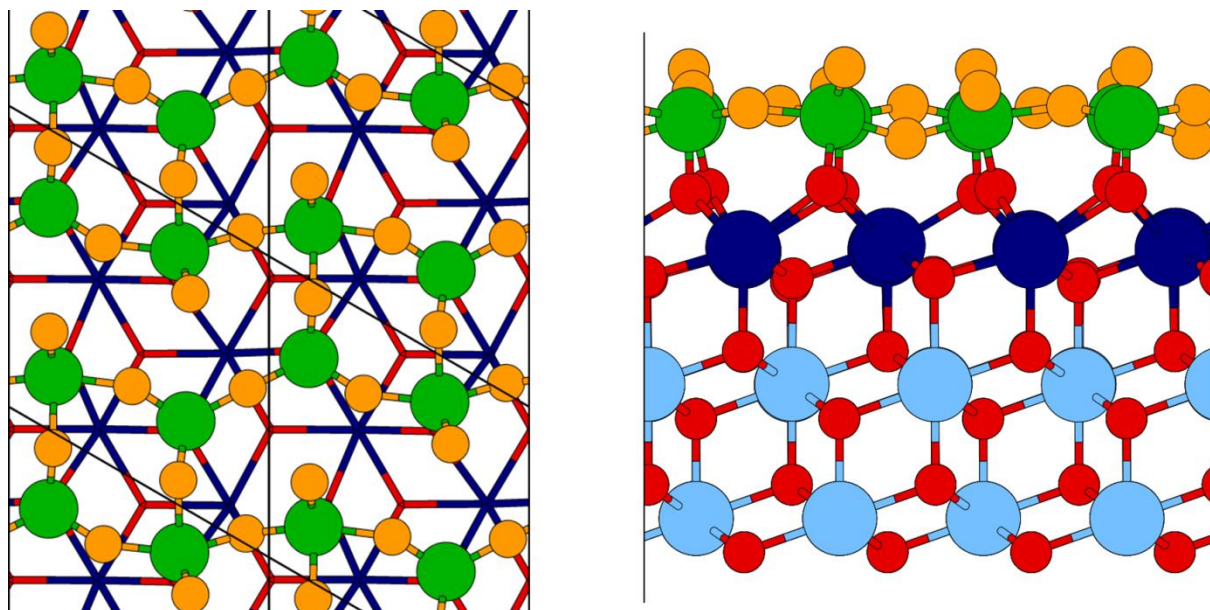


Figure S2 VO₂-ML-b, i.e. a VO₂ ML on CeO₂(111) with a different connection of its repeat units compared to the most stable structure (see Figure 2). For details and color code, see Figure 1. Black lines indicate primitive unit cells.

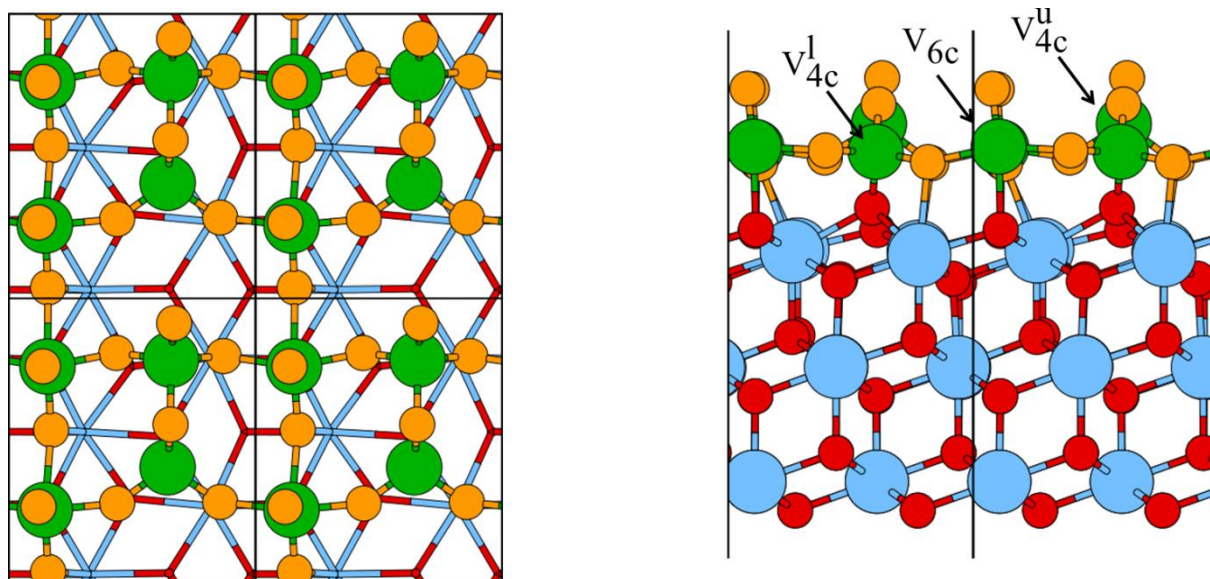


Figure S3 V₂O₅-ML-b, i.e. a V₂O₅ ML on CeO₂(111) with a different connection of its repeat units compared to the most stable structure (see Figure 5). For details and color code, see Figure 1. Black lines indicate primitive unit cells.

4. Total energies

Table S1 Total energies (dispersion-corrected PBE+U) for VO₂ oligomers as well as VO₂ and V₂O₅ MLs on the $p(4 \times 4)$ cell of CeO₂(111).

structure	total energy [eV]	coordinates on page
Ce ₄₈ O ₉₆	-1178.841216	S6-S7
Ce ₄₈ O ₉₅	-1171.871464	S7-S9
V/Ce ₄₈ O ₉₆	-1192.297766	S9-S11
VO/Ce ₄₈ O ₉₆	-1199.516040	S11-S13
VO ₂ /Ce ₄₈ O ₉₆	-1205.436656	S13-S14
VO ₃ /Ce ₄₈ O ₉₆	-1210.568784	S15-S16
V ₂ O/Ce ₄₈ O ₉₆	-1212.044535	S16-S18
V ₂ O ₂ /Ce ₄₈ O ₉₆	-1219.349522	S18-S20
V ₂ O ₃ /Ce ₄₈ O ₉₆	-1226.233673	S20-S22
V ₂ O ₄ /Ce ₄₈ O ₉₆	-1233.023802	S22-S23
V ₂ O ₅ /Ce ₄₈ O ₉₆	-1239.449187	S23-S25
V ₃ O ₂ /Ce ₄₈ O ₉₆	-1230.256091	S25-S27
V ₃ O ₃ /Ce ₄₈ O ₉₆	-1237.745835	S27-S29
V ₃ O ₄ /Ce ₄₈ O ₉₆	-1245.960838	S29-S31
V ₃ O ₅ /Ce ₄₈ O ₉₆	-1253.392202	S31-S33
V ₃ O ₆ /Ce ₄₈ O ₉₆	-1260.618283	S33-S34
V ₄ O ₈ /Ce ₄₈ O ₉₆	-1287.831046	S34-S36
V ₅ O ₁₀ /Ce ₄₈ O ₉₆	-1314.610220	S36-S38
V ₆ O ₁₂ /Ce ₄₈ O ₉₆	-1342.332911	S38-S40
V ₇ O ₁₄ /Ce ₄₈ O ₉₆	-1369.231843	S40-S42
V ₈ O ₁₆ /Ce ₄₈ O ₉₆	-1396.032260	S42-S44
V ₁₆ O ₃₂ /Ce ₄₈ O ₉₆ (VO ₂ -ML-a)	-1613.924365	S44-S46
V ₁₆ O ₃₂ /Ce ₄₈ O ₉₆ (VO ₂ -ML-b)	-1613.106925	S46-S49
V ₁₆ O ₃₂ /Ce ₄₈ O ₉₆ (VO ₂ -ML-c)	-1610.706366	S49-S51
V ₁₆ O ₃₁ /Ce ₄₈ O ₉₆	-1605.984657	S51-S53
V ₁₆ O ₄₀ /Ce ₄₈ O ₉₆ (V ₂ O ₅ -ML-a)	-1660.020220	S53-S56
V ₁₆ O ₄₀ /Ce ₄₈ O ₉₆ (V ₂ O ₅ -ML-b)	-1659.989623	S56-S58
V ₁₆ O ₃₉ /Ce ₄₈ O ₉₆	-1654.066772	S58-S60
V ₁₆ O ₃₈ /Ce ₄₈ O ₉₆	-1648.351920	S60-S63

Table S2 Optimized lattice parameters, employed k meshes, number of formula units per unit cell (f.u./u.c.), and total energies per unit cell of various bulk phases. The total energy of an isolated O₂ molecule ('hard' oxygen pseudopotential, plane wave kinetic energy cutoff of 1000 eV) is -10.052852 eV.

system	a ₀ [pm]	b ₀ [pm]	c ₀ [pm]	k mesh	f.u./u.c.	total energy [eV]
CeO ₂	549	549	549	10 × 10 × 10	1	-25.049161
V	299	299	299	12 × 12 × 12	1	-9.455177
V ₂ O ₃	548	548	548	8 × 8 × 8	2	-90.553772
VO ₂ (M1)	565	456	538	8 × 8 × 8	4	-106.055272
V ₂ O ₅	1165	354	447	2 × 6 × 6	2	-119.107582
CeVO ₄	743	743	655	6 × 6 × 6	2	-105.680464

5. x,y,z coordinates of optimized structures

Optimized structures are presented in VASP-style output (CONTCAR/POSCAR) below, containing the unit cell vectors and x,y,z coordinates of all atoms. For information on the structure of these files, we refer to the description given in the VASP online manual (http://cms.mpi.univie.ac.at/vasp/vasp/POSCAR_file.html).

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12.3189738143999676	-5.8192059665000038	3.5062484074000504	F	F	F
12.3189738143999676	-1.9397353222000042	3.5062484074000504	F	F	F
8.9592536831999681	3.8794706443000546	3.5062484074000504	F	F	F
8.9592536831999681	7.7589412886000559	3.5062484074000504	F	F	F
12.3189738143999676	1.9397353222000042	3.5062484074000504	F	F	F
12.3189738143999676	5.8192059665000038	3.5062484074000504	F	F	F

CeO₂-x (111)

1.0

13.4388805248000001	-7.7589412886000000	0.0000000000000000
0.0000000000000000	15.5178825772000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.0000000000000000

Ce O

48 95
Selective Dynamics
Cartesian

2.1924462992925879	-0.0233228543924258	10.5801420850557371	T	T	T
2.2185663426141371	3.8748287312155356	10.6196636556754509	T	T	T
5.5801114680143629	-1.9675318787283360	10.5977637490563446	T	T	T
5.5366041680296902	1.7811055535197124	10.6494180611200839	T	T	T
2.1978180917296353	7.7697747517389901	10.6000280730107193	T	T	T
2.2343177727044594	11.6481661345755612	10.5828971245479142	T	T	T
5.5253128904466484	5.9569115843469440	10.6546132878431479	T	T	T
5.5930163553002492	9.7288969983977971	10.6803893815360631	T	T	T
8.9915226132946753	-3.8830858735836014	10.5924713273676900	T	T	T
8.9805887322786333	-0.0456620477749059	10.5694614112120835	T	T	T
12.3264842634424721	-5.8262805802331643	10.5742732628091112	T	T	T
12.3242157029522996	-1.9358885173216551	10.5835379272751737	T	T	T
9.1052909526203898	3.87605088850560411	10.6593554617753696	T	T	T
8.9958197331972585	7.8075162853759181	10.5613363990098890	T	T	T
12.3473898019127670	1.9270160167958865	10.5822969530563817	T	T	T
12.3389906799981368	5.8284367088547215	10.5716887391056815	T	T	T
13.4376244169845052	7.7550763188978493	7.4219479737377814	T	T	T
0.0048092654494879	3.8781938452791649	7.4439180581305546	T	T	T
3.3554340675448344	13.5781923822295134	7.4395692985556598	T	T	T
3.3476522990172177	1.9464473874269526	7.4592046812419079	T	T	T
0.0022785273155988	7.7631494937492160	7.4304789395123301	T	T	T
0.0006504024160943	11.6356390846106184	7.4374002525279188	T	T	T
3.3483291150482057	5.8088997729393084	7.4635487851209010	T	T	T
3.3651477993074388	9.6974906408342854	7.4639198673136393	T	T	T
6.7134570881477913	11.6298869324482670	7.4595596397684316	T	T	T
6.7252797155430875	-0.0089566582040366	7.4484085607686348	T	T	T
10.0883331296664185	-5.8120248892191420	7.4237002237992948	T	T	T
10.0855035084433915	-1.9495543282032313	7.4301427287563273	T	T	T
6.7137880744331184	3.8807808869022815	7.3391378700825980	T	T	T
6.7208388933170422	7.7702699084343063	7.4686822347053372	T	T	T
10.0750996294999826	1.9315199074487985	7.4497021921175923	T	T	T
10.0719728962243718	5.8260116191174331	7.4460305010826771	T	T	T
1.1199067100000288	1.9397353228999972	4.2969520313999974	F	F	F
1.1199067100000288	5.8192059671999976	4.2969520313999974	F	F	F
4.4796268412000293	0.0000000007999446	4.2969520313999974	F	F	F
4.4796268412000293	3.8794706450999445	4.2969520313999974	F	F	F
1.1199067100000288	9.6986766114999963	4.2969520313999974	F	F	F
1.1199067100000288	13.5781472557999958	4.2969520313999974	F	F	F
4.4796268412000293	7.7589412893999441	4.2969520313999974	F	F	F
4.4796268412000293	11.6384119336999436	4.2969520313999974	F	F	F
7.8393469724000289	-1.9397353214000028	4.2969520313999974	F	F	F
7.8393469724000289	1.9397353228999972	4.2969520313999974	F	F	F
11.1990671036000293	-3.8794706435000550	4.2969520313999974	F	F	F
11.1990671036000293	0.0000000007999450	4.2969520313999974	F	F	F
7.8393469724000289	5.8192059671999967	4.2969520313999974	F	F	F
7.8393469724000289	9.6986766114999963	4.2969520313999974	F	F	F
11.1990671036000293	3.8794706450999445	4.2969520313999974	F	F	F
11.1990671036000293	7.7589412893999441	4.2969520313999974	F	F	F
1.0334995189082239	1.8052978944538993	11.3841123595454725	T	T	T
1.0142126514217493	5.9392768784356589	11.3955072378642530	T	T	T
4.4846426181447487	-0.0562090202743692	11.4484680704904989	T	T	T
4.8734973057078328	3.8574355897010730	11.1584766754720217	T	T	T
1.0682761453241776	9.7078726129393065	11.3913922852594638	T	T	T
1.0931803759893468	13.5757054642176538	11.3689828252005629	T	T	T
4.3916205681186593	7.6760569277046784	11.4881748178267671	T	T	T
4.3917850974078902	11.7811544729723856	11.4083464162531403	T	T	T
7.9066496264725341	-1.8879391378764572	11.3967384587096117	T	T	T
7.7496554019184947	2.1085976447807848	11.1797630039694589	T	T	T
11.1774230034133506	-3.8808091773039841	11.3648433768355694	T	T	T
11.1662604179087790	-0.0100202041511936	11.3685215181018471	T	T	T
7.7489868608621579	5.5777569140587433	11.2015268182235364	T	T	T
8.0356803860096040	9.6767023991556869	11.4064318297582670	T	T	T
11.2262511718278386	3.8835692669355542	11.4262406890071464	T	T	T
11.1855609535363740	7.7600941738263156	11.3625399422560047	T	T	T
13.4140760518841748	7.7199807189110423	9.7475273186992535	T	T	T
13.3977738000214028	-3.8818275521726666	9.7783362117498793	T	T	T
3.3322075171533587	-1.9102759013568931	9.7551844499207991	T	T	T
3.3734636490619887	1.8362876874330420	9.8025535538762725	T	T	T
13.4097723143298388	0.0342300656575105	9.7539751186916099	T	T	T
13.4283981206549683	3.8811096482869782	9.7746571530329120	T	T	T
3.3479956753057918	5.8803178510325678	9.7793573836719094	T	T	T
3.2972864226792096	9.7052131130156116	9.7983494047616890	T	T	T
6.7579629597463731	-3.8257803110943205	9.8125063373859849	T	T	T
6.6987881634136421	-0.0528628608295678	9.7879667592462045	T	T	T
10.1148506170709140	-5.8324860238944796	9.7358358925721706	T	T	T
10.0811888682461284	-1.9308615875229371	9.7584484439852304	T	T	T
6.7373915038681265	7.7541177928684668	9.8103351486399575	T	T	T
10.1302341494757275	1.9442236334347855	9.7922682229968174	T	T	T
10.1262332452430996	5.8122834050604677	9.7882744763753227	T	T	T
2.2173083023866860	0.0030984313304576	8.2126399726706740	T	T	T
2.2555204026207578	3.8615653619505714	8.2183013363887163	T	T	T
5.5865016255696229	-1.9470991320911477	8.2303539006172439	T	T	T
5.7035890461147973	2.0834166910771121	8.3705684990686198	T	T	T
2.2252491481767738	7.7622224071413113	8.2243579688147150	T	T	T
2.2346794976969102	11.6461515561774238	8.2380928348018188	T	T	T
5.6902734741984302	5.6659015567409057	8.3659261710313544	T	T	T

5.5982475766542921	9.7050763918524297	8.2109274254121321	T	T	T
8.9686107618627258	-3.8845461202556462	8.2308323275682902	T	T	T
8.9505852411553128	0.0160506393919446	8.2565516500453473	T	T	T
12.3370783638023234	-5.8277880557837900	8.2140765989596023	T	T	T
12.3220678949454410	-1.9330559906100948	8.2247263447401977	T	T	T
8.7758562238127489	3.8748564907525207	8.3811109614245769	T	T	T
8.9601018118471281	7.7463883225144041	8.2483470999494202	T	T	T
12.3139932338264018	1.9532543255068200	8.2163629663818316	T	T	T
12.3119020398849432	5.8033740461754961	8.2141950534694068	T	T	T
1.1332867804917861	1.9414784423000597	6.6252746729358423	T	T	T
1.1314304112010325	5.8151089515652972	6.6361885832535750	T	T	T
4.5117714332995087	0.0520430800987963	6.6742364331704946	T	T	T
4.4872678871318108	3.8743548220999076	6.6159613956304311	T	T	T
1.1205752594431349	9.7060570350059034	6.6288726247490191	T	T	T
1.1181905208551308	13.5702109453795625	6.6220860459420789	T	T	T
4.5082609086674861	7.7020740824844722	6.6804763761093255	T	T	T
4.4716983771227170	11.6422486239889302	6.6320428530190538	T	T	T
7.8382642535556375	-1.9234008470239772	6.6438540587119057	T	T	T
7.8423857362800993	1.9361050791170396	6.6134115782703100	T	T	T
11.2006144080565093	-3.8774640388651660	6.6278639854072079	T	T	T
11.1797015516378018	0.0103244326024772	6.6361796111725475	T	T	T
7.8427060057773206	5.8186712494786397	6.6175786834539148	T	T	T
7.8439975400831425	9.6829250500640587	6.6405784499337184	T	T	T
11.1264722842223112	3.8779703520038558	6.6657835423262952	T	T	T
11.1829531763881249	7.7453221358985536	6.6310681370599243	T	T	T
0.0000000000000000	0.0000000000000000	5.0875064657999340	F	F	F
0.0000000000000000	3.8794706443000000	5.0875064657999340	F	F	F
3.3597201312000000	-1.9397353221000511	5.0875064657999340	F	F	F
3.3597201312000000	1.9397353221000511	5.0875064657999340	F	F	F
0.0000000000000000	7.7589412886000000	5.0875064657999340	F	F	F
0.0000000000000000	11.6384119329000004	5.0875064657999340	F	F	F
3.3597201312000000	5.8192059664999487	5.0875064657999340	F	F	F
3.3597201312000000	9.6986766107999483	5.0875064657999340	F	F	F
6.7194402624000000	-3.8794706443000000	5.0875064657999340	F	F	F
6.7194402624000000	0.0000000000000000	5.0875064657999340	F	F	F
10.0791603936000005	9.6986766107000513	5.0875064657999340	F	F	F
10.0791603936000005	-1.9397353221999492	5.0875064657999340	F	F	F
6.7194402624000000	3.8794706443000000	5.0875064657999340	F	F	F
6.7194402624000000	7.7589412886000009	5.0875064657999340	F	F	F
10.0791603936000005	1.9397353221000504	5.0875064657999340	F	F	F
10.0791603936000005	5.8192059664999478	5.0875064657999340	F	F	F
2.2398134211999712	-0.0000000007999443	3.5062484075999838	F	F	F
2.2398134211999712	3.8794706435000554	3.5062484075999838	F	F	F
5.5995335523999712	-1.9397353228999972	3.5062484075999838	F	F	F
5.5995335523999712	1.9397353214000033	3.5062484075999838	F	F	F
2.2398134211999712	7.7589412878000550	3.5062484075999838	F	F	F
2.2398134211999712	11.6384119321000554	3.5062484075999838	F	F	F
5.5995335523999712	5.8192059657000046	3.5062484075999838	F	F	F
5.5995335523999712	9.6986766100000033	3.5062484075999838	F	F	F
8.9592536835999717	-3.8794706450999450	3.5062484075999838	F	F	F
8.9592536835999717	-0.0000000007999450	3.5062484075999838	F	F	F
12.3189738147999712	-5.8192059671999976	3.5062484075999838	F	F	F
12.3189738147999712	-1.9397353228999972	3.5062484075999838	F	F	F
8.9592536835999717	3.8794706435000545	3.5062484075999838	F	F	F
8.9592536835999717	7.7589412878000541	3.5062484075999838	F	F	F
12.3189738147999712	1.9397353214000042	3.5062484075999838	F	F	F
12.3189738147999712	5.8192059657000037	3.5062484075999838	F	F	F

V/CeO₂ (111)

1.0		
13.4388805250000001	-7.7589412890000000	0.0000000000000000
0.0000000000000000	15.5178825770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.0000000000000000

Ce O V

48 96 1

Selective Dynamics

Cartesian

1.9916802539189733	0.0092868572091904	10.5410946621523056	T	T	T
2.0525073692778855	3.8689942811885452	10.6765329169248258	T	T	T
5.7187730828797401	-2.1561298085036107	10.5537850157083728	T	T	T
5.6730214243861870	2.0341833450458275	10.5359579283529836	T	T	T
2.2311847462397494	7.7700162820762815	10.6724752902125886	T	T	T
2.2179477112205657	11.6350103530004372	10.6041215853902031	T	T	T
5.5898361085534063	5.9072108085786574	10.6233769479859195	T	T	T
5.5996962546267488	9.6651016986082023	10.6038313946963001	T	T	T
9.0025658054253110	-3.9022481797659418	10.6095998532201321	T	T	T
9.0174526607475229	-0.1213032919812651	10.7036452397754687	T	T	T
12.2636965328564607	-5.7941446906020015	10.5884562713292922	T	T	T
12.3313844944041602	-1.9064219163285658	10.6140779992571765	T	T	T
9.0894490329460798	3.8836951266716522	10.4989728912638611	T	T	T
9.0342312413386647	7.9091297668312777	10.5475607349200260	T	T	T
12.3476593185245420	1.9201440466759152	10.5862332563327062	T	T	T
12.2861780975232051	5.8107896060767557	10.5651172621558942	T	T	T
13.4086592001601819	7.7689724350092213	7.3901515265542779	T	T	T
13.4374526370965839	-3.8784859516308035	7.4342249904215265	T	T	T
3.3695537355111487	-1.9205134388018357	7.4527474385034225	T	T	T
3.3512815115877528	1.9461399026522472	7.4358944413116594	T	T	T

0.0132179104248148	7.7522209177858450	7.4550355183434087	T	T	T
13.4236074699627732	3.8872244974576446	7.4341653740846274	T	T	T
3.3620566448378111	5.8058144933606295	7.4890698987859565	T	T	T
3.3684118228722895	9.6806727021449426	7.4597795192661200	T	T	T
6.7341009078362433	11.6097467473737179	7.4029465932076599	T	T	T
6.7245453385250267	-0.0086523361412447	7.4445281559521703	T	T	T
10.0867443616159456	-5.7984174610141359	7.3921215480318798	T	T	T
10.0774627681990587	-1.9366434104204591	7.4473614119916220	T	T	T
6.7220546635591063	3.8928058411865814	7.4177419450893618	T	T	T
6.7210586839499804	7.7447668163579451	7.4313732971761075	T	T	T
10.0708512252084947	1.9190228739408601	7.4366208049114144	T	T	T
10.0722068141700198	5.8305930243080200	7.4029220727355636	T	T	T
1.1199067104122100	1.9397353221375813	4.2969520308960236	F	F	F
1.1199067104122100	5.8192059663875817	4.2969520308960236	F	F	F
4.4796268416622098	-0.0000000001589471	4.2969520308960236	F	F	F
4.4796268416622098	3.8794706440910529	4.2969520308960236	F	F	F
1.1199067104122100	9.6986766106375839	4.2969520308960236	F	F	F
1.1199067104122100	13.5781472548875826	4.2969520308960236	F	F	F
4.4796268416622098	7.7589412883410516	4.2969520308960236	F	F	F
4.4796268416622098	11.6384119325910511	4.2969520308960236	F	F	F
7.8393469729122103	-1.9397353224710256	4.2969520308960236	F	F	F
7.8393469729122103	1.9397353218875812	4.2969520308960236	F	F	F
11.1990671041622107	-3.8794706446589475	4.2969520308960236	F	F	F
11.1990671041622107	-0.0000000004089475	4.2969520308960236	F	F	F
7.8393469729122103	5.8192059661375826	4.2969520308960236	F	F	F
7.8393469729122103	9.6986766103875812	4.2969520308960236	F	F	F
11.1990671041622107	3.8794706438410511	4.2969520308960236	F	F	F
11.1990671041622107	7.7589412880910515	4.2969520308960236	F	F	F
0.8996021009918482	1.7866320443821688	11.4457312436922365	T	T	T
0.8961331045042097	5.8146906475278195	11.4704238099404847	T	T	T
5.3073331704447231	3.9029592760479712	12.1966766639806963	T	T	T
1.0609400436694012	9.8791466637129037	11.4127618614029132	T	T	T
1.0182280810086322	13.5994139463248942	11.3585623948139585	T	T	T
4.5972153310254287	7.9399938195771620	11.4255703093999301	T	T	T
4.5304233155409435	11.6191440122717662	11.3852064631914374	T	T	T
7.8141592646412503	-2.1714969841111205	11.4586136687241265	T	T	T
7.7486708643070452	2.5023963065284969	12.0365030418929564	T	T	T
11.1569177657390828	-3.9395123502041818	11.4142699151155256	T	T	T
11.3282021644526392	0.0296073186292771	11.4256173950894748	T	T	T
7.770185847052247	5.2803248450322737	12.0365603740190039	T	T	T
7.9232698043851340	9.7049500751693003	11.3978166558652845	T	T	T
11.2216369881222526	3.9223980997578582	11.3132252642596711	T	T	T
11.17087114035274053	7.7823842124628735	11.3559221594958331	T	T	T
13.3616088114739817	7.7314907552300953	9.7185309912158573	T	T	T
13.3577905957229337	-3.9045297095115621	9.7618251969846863	T	T	T
3.4805639115411320	-1.7015533999265764	10.0377558301165823	T	T	T
3.3970262115668062	1.7884385819928998	10.1380391988755338	T	T	T
13.4165169302064628	0.0553051888545149	9.7398509808366498	T	T	T
0.0007312411637880	11.6659821062562887	9.7367963553098917	T	T	T
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12.3210628865742802	-1.9273021655451030	8.2220580125403178	T	T	T
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VO/CeO2 (111)

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Selective Dynamics

Cartesian

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Ce O V			
48 98 1			
Selective Dynamics			
Cartesian			
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5.6020847291479567	1.9643823892047001	8.2470403158233374	T	T	T
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2.2451244214915937	11.6526106528964650	8.2541350628710504	T	T	T
5.6036819902640307	5.8178127917893594	8.2403785352889845	T	T	T
5.5945792337905900	9.6919445386764558	8.2258645420298038	T	T	T
8.9675602132464078	-3.8785458097008862	8.2258641236145476	T	T	T
8.9443035850425545	0.0025022704854605	8.2541326248217572	T	T	T
12.3181080497814133	-5.8234944939043283	8.2403780772458592	T	T	T
12.3133080357915539	-1.9216138664869487	8.2235943046642515	T	T	T
8.9522439193241059	3.8813860826546982	8.2414002845774821	T	T	T
8.9599614561793732	7.7577161797030518	8.2355083712236326	T	T	T
12.3213539782986263	1.9356124582772356	8.2286733215716179	T	T	T
12.3208193227168561	5.8262296478286650	8.2413983708353715	T	T	T
1.1232611807776007	1.9453184568972515	6.6393849881675120	T	T	T
1.1289497015044554	5.8035441416269276	6.6426627446424407	T	T	T
4.4800199595993355	-0.0006794718260665	6.6591421104914161	T	T	T
4.4731138770964272	3.8793571648136513	6.6393859194679310	T	T	T
1.1210368179121049	9.7105735500650461	6.6305355660169951	T	T	T
1.1223483610215974	13.5788727467283259	6.6379973505562857	T	T	T
4.4780309084876357	7.7532990135981770	6.6318368069911102	T	T	T
4.4763342579177738	11.6427444341116288	6.6343306474765127	T	T	T
7.8372397251935073	-1.9347173392691812	6.6343303042562978	T	T	T
7.8374967803328994	1.9379842140292229	6.6379972322944365	T	T	T
11.2047507657040608	-3.8809111304513735	6.6318358341084345	T	T	T
11.1881980560725989	0.0049743911105278	6.6305327251631585	T	T	T
7.8386507616578589	5.8187557371481509	6.6306634920418466	T	T	T
7.8407146336980773	9.6963078868123063	6.6273317502348856	T	T	T
11.1973748268535811	3.8824003777182767	6.6359129740454961	T	T	T
11.1998051991686829	7.7593188287483645	6.6306640008488396	T	T	T
0.0000000000000000	0.0000000000000000	5.0875064649998913	F	F	F
0.0000000000000000	3.8794706443000000	5.0875064649998913	F	F	F
3.3597201312000000	13.5781472549999425	5.0875064649998913	F	F	F
3.3597201312000000	1.9397353221999494	5.0875064649998913	F	F	F
0.0000000000000000	7.7589412886000000	5.0875064649998913	F	F	F
0.0000000000000000	11.6384119329000004	5.0875064649998913	F	F	F
3.3597201312000000	5.8192059664999487	5.0875064649998913	F	F	F
3.3597201312000000	9.6986766107999483	5.0875064649998913	F	F	F
6.7194402624000000	-3.8794706443000000	5.0875064649998913	F	F	F
6.7194402624000000	0.0000000000000000	5.0875064649998913	F	F	F
10.0791603936000005	9.6986766107000513	5.0875064649998913	F	F	F
10.0791603936000005	-1.9397353221999492	5.0875064649998913	F	F	F
6.7194402624000000	3.8794706443000000	5.0875064649998913	F	F	F
6.7194402624000000	7.7589412886000009	5.0875064649998913	F	F	F
10.0791603936000005	1.9397353221999483	5.0875064649998913	F	F	F
10.0791603936000005	5.8192059664999478	5.0875064649998913	F	F	F
2.2398134207999680	0.0000000000000551	3.5062484074000504	F	F	F
2.2398134207999680	3.8794706443000551	3.5062484074000504	F	F	F
5.5995335519999685	-1.9397353222000040	3.5062484074000504	F	F	F
5.5995335519999685	1.9397353222000047	3.5062484074000504	F	F	F
2.2398134207999680	7.7589412886000542	3.5062484074000504	F	F	F
2.2398134207999680	11.6384119329000555	3.5062484074000504	F	F	F
5.5995335519999685	5.8192059665000038	3.5062484074000504	F	F	F
5.5995335519999685	9.6986766108000033	3.5062484074000504	F	F	F
8.9592536831999681	-3.8794706442999449	3.5062484074000504	F	F	F
8.9592536831999681	0.0000000000000551	3.5062484074000504	F	F	F
12.3189738143999676	-5.8192059665000038	3.5062484074000504	F	F	F
12.3189738143999676	-1.9397353222000042	3.5062484074000504	F	F	F
8.9592536831999681	3.8794706443000546	3.5062484074000504	F	F	F
8.9592536831999681	7.7589412886000559	3.5062484074000504	F	F	F
12.3189738143999676	1.9397353222000042	3.5062484074000504	F	F	F
12.3189738143999676	5.8192059665000038	3.5062484074000504	F	F	F
4.7039925250627510	-0.3885820931786683	14.4789725823905933	T	T	T
5.0357332123355443	2.0148259262116537	12.9888473042465797	T	T	T
2.4566986940606017	0.5257843932989450	12.9888554604347330	T	T	T
4.195003056853673	0.4929904287941382	13.1813695015877990	T	T	T

V2O/CeO2 (111)

1.0

13.4388805248000001	-7.7589412886000000	0.0000000000000000
0.0000000000000000	15.5178825772000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.0000000000000000

Ce O V

48 97 2

Selective Dynamics

Cartesian

2.0160440445685959	-0.0100729235702377	10.6340126996429838	T	T	T
2.1617927406443300	3.8161577002973823	10.6963330169659478	T	T	T
5.6585432539004898	-2.0882639695653284	10.6267109795105057	T	T	T
5.7403488810781393	2.0474650318935690	10.5986701006932957	T	T	T
2.2061474483620116	7.8166958790313759	10.6082625785500184	T	T	T
2.2394061292527643	11.6531773088045458	10.6142018274140266	T	T	T
5.6517104746995823	5.9271745628031773	10.4030743344499612	T	T	T
5.6230993953764017	9.7539467243194125	10.6987724538086830	T	T	T
8.9692813073170345	-3.9297871033140304	10.6023076654771469	T	T	T

9.0279039977077886	-0.2018750361252053	10.5764405260577039	T T T
12.2821769868123631	-5.8053560041955503	10.6235247415270582	T T T
12.1314955429877394	-1.9594637920372806	10.5166293387571379	T T T
9.0577678270146986	3.9082725132944418	10.6425574296360548	T T T
9.0652762629590793	7.8988480384679365	10.5925939459340395	T T T
12.3386193117336589	1.9458819252638433	10.6220509099346287	T T T
12.3193833342833923	5.7793074639539874	10.5797428875231407	T T T
13.4329118945033041	-7.7466022701637307	7.4268139231859482	T T T
0.0183490958593617	3.8775731545235717	7.4389851663709274	T T T
3.3660036843250007	-1.9215597287249537	7.4923598685051704	T T T
3.3593879141386753	1.9364191257312477	7.3970082994441588	T T T
13.4343357636582681	-0.0170116168684116	7.4469567020117786	T T T
13.4383272672661693	3.8779041975910378	7.4364917885880146	T T T
3.3523184518185110	5.8121714594602336	7.4488290896521745	T T T
3.3736947882571169	9.6911293073155527	7.4631872100211138	T T T
6.7134260478994818	11.6245264590166979	7.4303141597200080	T T T
6.7042437063460705	-0.0035427478724261	7.4261719833672206	T T T
10.0907386664207994	-5.8075308803169552	7.4015771398942833	T T T
10.0545566799768800	-1.9617546685677434	7.3638174656040229	T T T
6.7357722278457119	3.8870244954300586	7.4098858643161787	T T T
6.7376925669460501	7.7984766121507771	7.4111054918881836	T T T
10.0585335359808408	1.9295606913167251	7.4577939738202019	T T T
10.0735828310845008	5.8189685136830986	7.4404375732676939	T T T
1.1199067099519970	1.9397353229259637	4.2969520313999974	F F F
1.1199067099519970	5.8192059672259644	4.2969520313999974	F F F
4.4796268411519966	0.0000000007759637	4.2969520313999974	F F F
4.4796268411519966	3.8794706450759646	4.2969520313999974	F F F
1.1199067099519970	9.6986766115259648	4.2969520313999974	F F F
1.1199067099519970	13.5781472558259644	4.2969520313999974	F F F
4.4796268411519966	7.7589412893759642	4.2969520313999974	F F F
4.4796268411519966	11.6384119336759646	4.2969520313999974	F F F
7.8393469723519980	-1.9397353213740369	4.2969520313999974	F F F
7.8393469723519980	1.9397353229259640	4.2969520313999974	F F F
11.1990671035519984	-3.8794706435240367	4.2969520313999974	F F F
11.1990671035519984	0.0000000007759642	4.2969520313999974	F F F
7.8393469723519980	5.8192059672259635	4.2969520313999974	F F F
7.8393469723519980	9.6986766115259631	4.2969520313999974	F F F
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11.1990671035519984	7.7589412893759633	4.2969520313999974	F F F
0.8158313011064924	1.9508139097589914	11.4653854261032855	T T T
2.2189707132413710	5.7414520888471277	12.3630817904015196	T T T
5.0149714554575011	4.7553898552300566	12.6293498732319716	T T T
0.9836512581803369	9.7847309786655465	11.3797525714669128	T T T
0.9690622802982295	13.4618524990081276	11.4168657565643059	T T T
4.3653684843798528	7.4829064205972147	12.0025156504321799	T T T
4.3183515911811785	11.6332686673976156	11.4823148971864502	T T T
8.0478535776404776	-2.0359117698333336	11.4560133068601608	T T T
7.3193869808116983	2.9129213432285566	12.3780661699025814	T T T
11.1454102361678871	-3.8569388405852822	11.3767734499136424	T T T
11.1358392047549888	-0.1307988942731129	11.4210951055910570	T T T
7.6792165588952832	5.6314236473886368	12.0234798206323177	T T T
8.0451785984671993	9.7157651232799296	11.4688007321949605	T T T
11.3392482080975494	3.8416632330043186	11.3706580574441176	T T T
11.1642100385049847	7.8323927869125978	11.4177335293869167	T T T
13.3271744377410073	7.7205925141292644	9.7450463345902030	T T T
0.0183931624119335	4.1051096933673730	9.8808318770741916	T T T
3.3828844175899118	-1.8367883626927044	9.8632903338709284	T T T
3.5114459734167718	1.9176229246378687	10.4305266797781702	T T T
13.4141156559423997	-0.1796561195128206	9.9005313940965110	T T T
13.4290122807068197	3.8651213172387440	9.7013246471371506	T T T
3.3906681108953087	5.7595872807080104	9.7534154622729901	T T T
3.3834878348165760	9.6429885319894222	9.8128178283957492	T T T
6.7550110544093576	11.6019335665002323	9.8064766419101570	T T T
6.7737927345422433	0.0922447174999954	10.1585093080729276	T T T
10.1054389363285395	-5.8097947895599207	9.7357188725467108	T T T
10.0685470099073395	-1.9785721873897382	9.7030757694664267	T T T
6.7167412135389704	3.9382284183084360	9.7403907998338148	T T T
6.8336127094642212	7.7646374015503277	9.8507017645860522	T T T
9.8994314606648040	1.8211271141675827	9.9392172881562733	T T T
9.9980551131643214	5.8985502428447365	9.8700195274968081	T T T
2.2380549371505820	0.1072710208822623	8.2485615436006636	T T T
2.2499873230408536	3.7311000149535340	8.2638944831159460	T T T
5.6553220199214662	-1.8945185787475012	8.2475032449083692	T T T
5.5756421682253876	1.9016239120604532	8.2312962447097675	T T T
2.1949830447811975	7.7544406210538135	8.1832480903050069	T T T
2.2851400699281652	11.6628765681778166	8.2748060023982397	T T T
5.6222152799831102	5.8591814110825302	8.0739558864238905	T T T
5.6231308212549624	9.6883660396313012	8.2001657261170280	T T T
8.9531982949225082	-3.8897249346565719	8.2013377239099778	T T T
8.8936920432849522	-0.0529194483807407	8.2514594082028623	T T T
12.3692658286591683	-5.7452529481341852	8.2622771645800341	T T T
12.2651242791383677	-1.9393003635546568	8.1817099482896634	T T T
9.0085362754182690	3.8654128183134491	8.1994277182129558	T T T
8.9858122280749679	7.7916715570588870	8.2116568711875146	T T T
12.2612242744829416	1.8613082603250275	8.3300532722561371	T T T
12.2619347145653883	5.7992059193150531	8.2305275899088972	T T T
1.1058020586317154	1.9384041749359104	6.5919401151431440	T T T
1.1171942782290882	5.7850824887842842	6.6524630270374612	T T T
4.4778824115935008	-0.0105782579431133	6.6280638703499459	T T T

4.4774593183185942	3.8609442008626731	6.6279173240530644	T	T	T
1.0853120324398866	9.7125663254073267	6.6568203548368396	T	T	T
1.1257083846113691	13.5923467940702221	6.6703749931584015	T	T	T
4.4623510423550652	7.7769852835241311	6.6252921317880631	T	T	T
4.4850384920605375	11.6650102855538869	6.6532634240788324	T	T	T
7.8306252319584342	-1.9391507140239823	6.6020091098466080	T	T	T
7.8364263020487988	1.9241893901259965	6.6409982136497208	T	T	T
11.2013742217929426	-3.8862031494246212	6.6068669402163573	T	T	T
11.1718639999566989	0.0109622996686509	6.6272628119659123	T	T	T
7.8723688708818793	5.8191605067485268	6.6224356207415926	T	T	T
7.8517565703756995	9.7065714892873665	6.6064981420541482	T	T	T
11.2172862576708106	3.8394629307142250	6.6347725716850974	T	T	T
11.2192725360803252	7.7801698165805142	6.6326302330630300	T	T	T
0.0000000000000000	0.0000000000000000	5.0875064657999340	F	F	F
0.0000000000000000	3.8794706443000000	5.0875064657999340	F	F	F
3.3597201312000000	-1.9397353221500000	5.0875064657999340	F	F	F
3.3597201312000000	1.9397353221500000	5.0875064657999340	F	F	F
0.0000000000000000	7.7589412886000000	5.0875064657999340	F	F	F
0.0000000000000000	11.6384119329000004	5.0875064657999340	F	F	F
3.3597201312000000	5.8192059664500002	5.0875064657999340	F	F	F
3.3597201312000000	9.6986766107500006	5.0875064657999340	F	F	F
6.7194402624000000	-3.8794706443000000	5.0875064657999340	F	F	F
6.7194402624000000	0.0000000000000000	5.0875064657999340	F	F	F
10.0791603936000005	-5.8192059664500002	5.0875064657999340	F	F	F
10.0791603936000005	-1.9397353221500002	5.0875064657999340	F	F	F
6.7194402624000000	3.8794706443000000	5.0875064657999340	F	F	F
6.7194402624000000	7.7589412886000009	5.0875064657999340	F	F	F
10.0791603936000005	1.9397353221499998	5.0875064657999340	F	F	F
10.0791603936000005	5.8192059664500002	5.0875064657999340	F	F	F
2.2398134212480030	-0.0000000007759640	3.5062484075999838	F	F	F
2.2398134212480030	3.8794706435240363	3.5062484075999838	F	F	F
5.5995335524480030	-1.9397353229259644	3.5062484075999838	F	F	F
5.5995335524480030	1.9397353213740356	3.5062484075999838	F	F	F
2.2398134212480030	7.7589412878240376	3.5062484075999838	F	F	F
2.2398134212480030	11.6384119321240362	3.5062484075999838	F	F	F
5.5995335524480030	5.8192059656740369	3.5062484075999838	F	F	F
5.5995335524480030	9.6986766099740365	3.5062484075999838	F	F	F
8.9592536836480026	-3.8794706450759642	3.5062484075999838	F	F	F
8.9592536836480026	-0.0000000007759642	3.5062484075999838	F	F	F
12.3189738148480021	-5.8192059672259635	3.5062484075999838	F	F	F
12.3189738148480021	-1.9397353229259640	3.5062484075999838	F	F	F
8.9592536836480026	3.8794706435240371	3.5062484075999838	F	F	F
8.9592536836480026	7.7589412878240367	3.5062484075999838	F	F	F
12.3189738148480021	1.9397353213740374	3.5062484075999838	F	F	F
12.3189738148480021	5.8192059656740369	3.5062484075999838	F	F	F
7.2117096019537534	4.6168493004180933	14.6203014064120023	T	T	T
3.7190818047612209	6.5520917675084682	14.5917247473229601	T	T	T
6.8298457652735793	4.4643001863787077	13.0564689219093317	T	T	T
3.7914785290567976	6.1370599245274793	13.0312627958665530	T	T	T

V2O2/CeO2 (111)

1.0		
13.4388805248000001	-7.7589412886000000	0.0000000000000000
0.0000000000000000	15.5178825772000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.0000000000000000

Ce O V

48 98 2

Selective Dynamics

Cartesian

2.2148311927723654	-0.0332674612623125	10.5807039181362885	T	T	T
2.1688654257162394	3.8390194822900976	10.6136561671530920	T	T	T
5.5466226264825620	-1.9481456167471272	10.6152863025197153	T	T	T
5.5891250151275269	1.8349829485881681	10.6168309373728533	T	T	T
2.2131239955653070	7.8275867831945174	10.6175193230292901	T	T	T
2.2273907020217281	11.6598845642315343	10.5637773184013462	T	T	T
5.6582154828751827	5.8901057198924756	10.4094170709785470	T	T	T
5.6583256245708924	9.8100401439924010	10.6745119404721276	T	T	T
8.9525515862504470	-3.8938384825931474	10.5969153374315255	T	T	T
9.020375305804833	-0.1813583570407378	10.5480154001311117	T	T	T
12.3508479316549344	-5.8301356140777250	10.6012304402781918	T	T	T
12.1316878720059513	-1.9621310413450406	10.5338402587304891	T	T	T
9.0051912630408850	3.8983099639446808	10.6380503514471254	T	T	T
9.0792522057430176	7.9280007350342689	10.5602820077680981	T	T	T
12.3248474746716195	1.9615400927757785	10.6250302484960297	T	T	T
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13.4372745870867121	-0.0134068328425174	7.4451578433875474	T	T	T
13.4337536566365241	3.8715431287525277	7.4283062355881739	T	T	T
3.3510881687925513	5.8210600454356793	7.4392716129709449	T	T	T
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7.7145408491366894	11.6359230036255603	7.4412510678575270	T	T	T
6.7120959033777599	0.0040459195886196	7.4299532051614907	T	T	T
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10.0630078504568399	-1.9552909401509089	7.3658420291319224	T	T	T

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V203/CeO2 (111)

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Ce O V

48 99 2

Selective Dynamics

Cartesian

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6.7671846227018966	7.5510010079754206	9.9646956512200351	T T T
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1.1243640715657883	13.5665698686794194	6.6280500097933741	T T T
4.4566148767495202	7.7646103509507762	6.6400574156907801	T T T
4.4947044325299244	11.6211475557681343	6.6661926963495004	T T T
7.8363585879422208	-1.9590427492205422	6.6233617044246742	T T T
7.8283247529811710	1.9289710322767926	6.6392039321815330	T T T
11.1895004735676000	-3.8845408052593262	6.6261318550747825	T T T
11.2054523701685174	-0.0151354996273225	6.6467977494370150	T T T
7.8231616153940831	5.8476344944173038	6.6318454466466639	T T T
7.8592527242177974	9.7316058096849964	6.6487788789911457	T T T
11.2194528019849606	3.8909057716147348	6.6367498168182975	T T T
11.2012348678770461	7.7661192020780083	6.6208753552763753	T T T
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0.0000000000000000	3.8794706442000511	5.0875064649998913	F F F
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5.5995335521000111	-1.9397353224000409	3.5062484074000504	F F F
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8.9592536832999752	-0.0000000003000347	3.5062484074000504	F F F
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9.0735160803321300	3.2778180794150993	13.8752121899407506	T T T
6.1953950792405621	3.2804561020347145	14.1448400785595343	T T T
11.8583637235734916	2.7600365076905815	14.3539240826550838	T T T
7.4423965491853599	3.4595728836423092	13.1262586385649875	T T T
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V2O4/CeO2 (111)

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Ce O V

48 100 2

Selective Dynamics

Cartesian

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4.71713223519941382	2.6456819233033686	10.6812443007791931	T T T
4.7679583050262373	6.4670044492025101	10.5706460538465503	T T T
1.3876608569610926	12.2388897024063557	10.5426309626432229	T T T
11.5471696781685953	2.5913516779933250	10.5605084888063327	T T T
1.4197338751285717	8.3841733861565846	10.5374295948391676	T T T
4.7637124562352051	10.2800319880884103	10.5761136336000074	T T T
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11.5112713442135224	-5.2345583060289975	10.5848766737958027	T T T
11.5000896861023705	6.4327720844427025	10.5721306311368526	T T T
4.6575643207893194	-1.4075429143653053	10.5736441102617924	T T T
8.2539710117882077	-3.4559311759052074	10.5336015208827405	T T T
8.2955866573616017	0.6654325778377839	10.5783708853013056	T T T
8.1312504693865950	8.3466026840700671	10.5794718219766377	T T T
5.9083367017507049	4.4900715685926809	7.4706089362747390	T T T
5.9069393086763355	8.3777173210776112	7.4223393178996240	T T T
9.2510360599893282	2.5779815101624184	7.4359081998672147	T T T
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5.9105435691332966	-3.2443830679305239	7.4301460111788025	T T T
5.9011053053171434	0.6197099875679601	7.4751522212789201	T T T
9.2688369513928812	-5.2235979223686346	7.3946158951928780	T T T
9.2475554673087590	-1.3224708561725818	7.4342492379788316	T T T
12.6136143792750470	0.6240670299284057	7.4265743414019809	T T T
12.6167313096409437	4.5058337849788046	7.4100987866086543	T T T
2.5419656407376228	6.4383977825389227	7.4297963982301507	T T T
2.5424746330415293	10.3264865970714581	7.4185856612645997	T T T
12.6128901191861491	-7.1412219550721465	7.4075107869354753	T T T
12.6171668652860784	-3.2701012657958621	7.4334243709052119	T T T
2.5348703104067605	-1.3083321285001208	7.4152713887754569	T T T
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12.5895263847291368	-7.1373777841102450	9.7457190366698203	T T T
3.0013439986761465	-0.0983271810792257	14.4321016078116156	T T T
10.5690240139046185	4.5199773736613391	11.3565809593849014	T T T
9.2917265537964298	6.5025608850442831	9.7696903363419736	T T T
0.2363703095425340	2.5274457185338970	11.3661108919118643	T T T
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7.0717543769277453	2.6471273328398999	11.7511055017981079	T T T
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5.2671650439675570	1.5640217141230051	13.7220060104522013	T T T
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5.8606591340809857	8.4095232151512693	9.7317730393034694	T	T	T
0.2681121104342681	6.4370821910223661	11.3563421226012800	T	T	T
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6.0470116103851428	-3.0743480680219530	9.9510154688271761	T	T	T
10.5069175178457570	0.5961469537806252	11.2637859285334976	T	T	T
5.9878432986396417	0.4256500625614574	10.0192014797945159	T	T	T
9.2805770173838056	-5.2437618965814572	9.7461620926817343	T	T	T
9.0553163148827629	-1.3669736100395511	9.9349024339575180	T	T	T
9.2483555216622939	2.5429134122755253	9.8163043726576227	T	T	T
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3.5910560342775302	12.1607550882398385	11.2204212735729705	T	T	T
2.5420306117833684	-1.2436096076888317	9.8052686362296271	T	T	T
7.0519908236488433	10.2845740386529876	11.3303264728983635	T	T	T
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8.1500202725100870	4.5059151194116414	8.1944538192535887	T	T	T
8.1261723013814962	8.3806702082073077	8.2127496660022992	T	T	T
11.4866133897084346	2.5585350159021063	8.2347877123370488	T	T	T
11.5048101323460461	6.4311668073533994	8.2113026921793200	T	T	T
8.1640601058211484	-3.3058569404009321	8.2300305451342410	T	T	T
8.1498247220443201	0.6161973194095172	8.2228849124267924	T	T	T
11.4999220599673500	-5.1953651506663983	8.2180560086220442	T	T	T
11.4138880951902060	-1.3208329698990147	8.3000243936838984	T	T	T
1.4205763375956824	8.3769414382593048	8.1791014633767229	T	T	T
1.4575843745527233	12.2830825260493164	8.2294218786568383	T	T	T
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4.8169488314178093	10.4201638379334476	8.2892541451934783	T	T	T
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1.4304773621730433	4.4995997738448006	8.2406046055522904	T	T	T
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4.8065131235679699	2.4899497005969873	8.2650441798129197	T	T	T
7.0077705744556003	6.4440823999837757	6.6310392449945645	T	T	T
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10.3796419840657723	-3.2493991319692159	6.6244716118923126	T	T	T
10.3783110080091188	0.6059727692456738	6.6311394432449093	T	T	T
0.2986610488641889	10.3291574380361872	6.6311131289988197	T	T	T
0.3033473733963886	14.1960108030082850	6.6148567198535364	T	T	T
3.6807833439852606	8.4084263272178124	6.6394509049509427	T	T	T
3.6722847012637931	12.2584844404788171	6.6150823287408596	T	T	T
0.3020953078231352	2.5674638850129536	6.6301842542611418	T	T	T
0.2663269136821103	6.4282180957733139	6.6446988918874341	T	T	T
3.6611466521369671	0.6161617522209317	6.6390526876006097	T	T	T
3.6665380152884017	4.4803465101064521	6.6493871273908693	T	T	T
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9.25972000000000282	6.4397349999999287	5.0875060000000039	F	F	F
5.90000000000000465	-3.2589420000000073	5.0875060000000039	F	F	F
5.90000000000000465	0.6205289999999315	5.0875060000000039	F	F	F
9.25972000000000282	-5.1986770000000222	5.0875060000000039	F	F	F
9.25972000000000282	-1.3192059999999737	5.0875060000000039	F	F	F
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12.6194400000000098	4.5000000000000231	5.0875060000000039	F	F	F
2.5402789999999911	6.4397349999999589	5.0875060000000039	F	F	F
2.5402789999999911	10.3192060000000065	5.0875060000000039	F	F	F
12.6194400000000098	-7.1384120000000388	5.0875060000000039	F	F	F
12.6194400000000098	-3.2589419999999638	5.0875060000000039	F	F	F
2.5402789999999911	-1.3192070000000273	5.0875060000000039	F	F	F
2.5402789999999911	2.5602640000000205	5.0875060000000039	F	F	F
8.1398129999999771	4.5000000000000373	3.5062479999999563	F	F	F
8.1398129999999771	8.3794709999999757	3.5062479999999563	F	F	F
11.4995340000000326	2.5602649999999469	3.5062479999999563	F	F	F
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8.1398129999999771	-3.2589419999999492	3.5062479999999563	F	F	F
8.1398129999999771	0.6205289999999897	3.5062479999999563	F	F	F
11.4995340000000326	-5.1986770000000391	3.5062479999999563	F	F	F
11.4995340000000326	-1.3192059999999906	3.5062479999999563	F	F	F
1.42037300000000148	8.3794699999999587	3.5062479999999563	F	F	F
1.42037300000000148	12.2589410000000054	3.5062479999999563	F	F	F
4.7800929999999964	6.4397350000000522	3.5062479999999563	F	F	F
4.7800929999999964	10.3192059999999906	3.5062479999999563	F	F	F
1.42037300000000148	0.6205289999999453	3.5062479999999563	F	F	F
1.42037300000000148	4.4999990000000212	3.5062479999999563	F	F	F
4.7800929999999964	-1.3192070000000433	3.5062479999999563	F	F	F
4.7800929999999964	2.5602640000000059	3.5062479999999563	F	F	F
4.1316337167845649	0.2090166738131662	13.3095003337334070	T	T	T
7.0303871583414788	1.7562394337120315	13.3123569799192047	T	T	T

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Ce O V			
48 101 2			
Selective Dynamics			
Cartesian			
8.1872094916453673	4.5908072549900512	10.5765535864950468	T T T
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1.3996164848972557	4.5038649345218991	10.5462148724546747	T T T
4.7180406954374403	2.6666033954277091	10.5579171759331718	T T T
4.7847690240287424	6.4586168553497636	10.5464114478306197	T T T
1.4226377644706887	12.2437753270001739	10.5745462521352156	T T T
11.5086787450093659	2.5491890494292759	10.5755097077635636	T T T
1.4231836791515777	8.3713933147001747	10.5443849251378108	T T T
4.7715715464327637	10.2734163732424726	10.5499468492465613	T T T
11.5410245614764957	-1.3364484426041496	10.5503634112721834	T T T
11.4848436382766597	-5.2007671439754937	10.5648440707290359	T T T
11.4970776221462234	6.4407298443782803	10.5661528373277100	T T T
4.8497382781629295	-1.4591522635950014	10.6655604914589848	T T T
8.1756702250713502	-3.3249348413000517	10.5518849818144069	T T T
8.2233212334627943	0.4870571033915434	10.6654069401080243	T T T
8.1466819565667947	8.3897281916556743	10.5646717553138672	T T T
5.9067806930196918	4.4979914814178237	7.4230465493859503	T T T
5.9029948486197430	8.3767954977274215	7.4160920903721621	T T T
9.2391404436851587	2.5472947182707646	7.4643616806367774	T T T
2.2638863837423973	6.4378236943807385	7.4155857026315815	T T T
5.9007771552080612	-3.2595918980700178	7.4294181818718794	T T T
5.9048720927891836	0.6112133396820409	7.4813672757086893	T T T
9.2618175193266659	-5.2038581604615093	7.4122390706162395	T T T
9.2586425464326784	-1.3211659090931880	7.4292259812319630	T T T
12.6197493789489403	0.6149442498887643	7.4262843520640605	T T T
12.6154073205718866	4.5051109146837049	7.4345641762348480	T T T
2.5417516136547005	6.4355908893734117	7.4180544668074901	T T T
2.5432500127162330	10.3151294143620529	7.4262124028968746	T T T
12.6173890198390879	-7.1436324283744845	7.4153393425378296	T T T
12.6189486510028672	-3.2636835651367715	7.4161053023509673	T T T
2.5601858433371092	-1.3089218140581504	7.4641724005995540	T T T
2.5374545991063355	2.5527073031534626	7.4232647049925191	T T T
7.0199070000000008	6.43973500000000371	4.2969519999999628	F F F
7.0199070000000008	10.3192059999999763	4.2969519999999628	F F F
10.3796269999999833	4.50000000000000204	4.2969519999999628	F F F
10.3796269999999833	8.3794709999999597	4.2969519999999628	F F F
7.0199070000000008	-1.3192059999999763	4.2969519999999628	F F F
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0.3004659999999645	2.5602640000000179	4.2969519999999628	F F F
0.3004659999999645	6.43973500000000664	4.2969519999999628	F F F
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3.66018600000000412	4.49999900000000221	4.2969519999999628	F F F
0.2677775568989040	14.2073193329421166	11.3126497227697929	T T T
4.7463885758957609	-1.0838978100520951	12.9116053430896436	T T T
12.5905163612854007	-7.1389963441782820	9.7578552539538688	T T T
2.8158107911219332	0.2747249193582950	14.3642505217216563	T T T
10.3856760658517668	4.5303383124320860	11.3134457324751505	T T T
9.2722073979155777	6.4626483856556973	9.7583625653677881	T T T
0.2771039163321301	2.5526667630824926	11.3172573725484860	T T T
2.5355553419250003	2.5445397261155147	9.7567953824656808	T T T
6.8705980194440253	2.9270347734983462	11.6981389602267143	T T T
7.9345380746539016	0.7601350319335936	12.9079788067081793	T T T
5.9148124493137724	4.4941174352467872	9.7561634593911908	T T T
5.2574698040649173	1.7116186532764623	13.7422383431810431	T T T
7.7215976973560476	3.0902208439102630	14.3906320849919407	T T T
3.6530379868621932	4.5101063176218466	11.3098652678078260	T T T
3.4230876755394064	0.9174798591159099	11.6812153535842853	T T T
7.0350062265224205	6.4554486088490384	11.3172391329436017	T T T
0.2954876064415161	10.3238534655824985	11.3357402578674904	T T T
3.6713563009677301	8.3489946560515307	11.3306438164479122	T T T
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12.6261542415366765	4.4853070098552434	9.7623418153404771	T T T
2.5404127266039049	6.4367633172993335	9.7551551582999210	T T T
2.5137686765941734	10.2683147943233486	9.7422509831125019	T T T
5.8932626221532010	8.3651334362618215	9.7511442228705842	T T T
0.3186575125054013	6.4135535831971096	11.3308447232399043	T T T
12.6333345437004692	-3.2617728769352325	9.7514581297571272	T T T
5.8808030095409087	-3.335592983745179	9.7677950553530728	T T T
10.5004424303499793	0.5925973265014877	11.2774229048708214	T T T
5.8529991093984579	0.7075463958913502	9.9911562720676308	T T T
9.2714754327662341	-5.2216333738072382	9.7419711892612053	T T T
9.3324779519270393	-1.3428955881245210	9.7686237435756045	T T T
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10.4095745363321956	-3.3113456702632655	11.3305015466095238	T T T
3.6209935117536727	12.1384352716220079	11.2761369982516744	T T T

2.6084880762928888	-1.2323925636101547	9.8697475785516264	T	T	T
7.0477745341581315	10.2658063189302098	11.3303967016557632	T	T	T
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11.4490292769269573	2.5511366879830764	8.2723823089717126	T	T	T
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8.1415267067217378	-3.2639467027047782	8.2270866392880642	T	T	T
8.1076116622206573	0.5869105084559809	8.2578648161370438	T	T	T
11.5028963204037442	-5.1983645371126137	8.2154208627069192	T	T	T
11.5201082281220692	-1.3204369005806091	8.2132358308908522	T	T	T
1.4287060214303386	8.3627288877814649	8.1988856216389241	T	T	T
1.4507905005610178	12.2955213233403384	8.2708097098287912	T	T	T
4.78350278205477319	6.4312650390429047	8.2263832638388035	T	T	T
4.7687399376624304	10.2996097487929514	8.2127532184576459	T	T	T
1.4005838439447738	0.6061627389379575	8.2415435293450976	T	T	T
1.4242352819377406	4.4920984438286178	8.2259960718396279	T	T	T
4.8242289678275307	-1.3072178705670929	8.2596230043879864	T	T	T
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7.0217656220116851	6.4299546500508242	6.6239502514621398	T	T	T
7.0195286469105334	10.3201099020064753	6.6243053051443859	T	T	T
10.3818701546992109	4.4897913744021647	6.6337489302610191	T	T	T
10.3818138607547947	8.3746634311274768	6.6217313924518937	T	T	T
7.0198503170953934	-1.3206620581933928	6.6297259916349640	T	T	T
7.0220134779122789	2.5539105149200134	6.6517654765643357	T	T	T
10.3780276370539024	-3.2587707341833516	6.6241734831444878	T	T	T
10.3666839358097675	0.6239905238051975	6.6410335141682797	T	T	T
0.2903140365167956	10.3345277267123485	6.6507212662222708	T	T	T
0.3070659255846171	14.1912064951847654	6.6338723266700121	T	T	T
3.6636379617363626	8.3731815737765434	6.6190315613352784	T	T	T
3.6628966328319441	12.2719345068078489	6.6414710276429432	T	T	T
0.3069832538874591	2.5531579969395430	6.6239303298623238	T	T	T
0.3028639644060863	6.4330829741113202	6.6190313180450469	T	T	T
3.6635745400030584	0.6148871733662395	6.6517891206306299	T	T	T
3.6655929237568134	4.4895885130563045	6.6283407624671975	T	T	T
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5.90000000000000465	-3.2589420000000073	5.0875060000000039	F	F	F
5.90000000000000465	0.6205289999999315	5.0875060000000039	F	F	F
9.25972000000000282	-5.1986770000000222	5.0875060000000039	F	F	F
9.25972000000000282	-1.3192059999999737	5.0875060000000039	F	F	F
12.6194400000000098	0.6205289999999746	5.0875060000000039	F	F	F
12.6194400000000098	4.5000000000000231	5.0875060000000039	F	F	F
2.5402789999999911	6.4397349999999589	5.0875060000000039	F	F	F
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12.6194400000000098	-7.1384120000000388	5.0875060000000039	F	F	F
12.6194400000000098	-3.2589419999999638	5.0875060000000039	F	F	F
2.5402789999999911	-1.3192070000000273	5.0875060000000039	F	F	F
2.5402789999999911	2.5602640000000205	5.0875060000000039	F	F	F
8.1398129999999771	4.5000000000000373	3.5062479999999563	F	F	F
8.1398129999999771	8.3794709999999757	3.5062479999999563	F	F	F
11.4995340000000326	2.5602649999999469	3.5062479999999563	F	F	F
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8.1398129999999771	-3.2589419999999492	3.5062479999999563	F	F	F
8.1398129999999771	0.6205289999999897	3.5062479999999563	F	F	F
11.4995340000000326	-5.1986770000000391	3.5062479999999563	F	F	F
11.4995340000000326	-1.3192059999999906	3.5062479999999563	F	F	F
1.4203730000000148	8.3794699999999587	3.5062479999999563	F	F	F
1.4203730000000148	12.2589410000000054	3.5062479999999563	F	F	F
4.7800929999999964	6.4397350000000522	3.5062479999999563	F	F	F
4.7800929999999964	10.3192059999999906	3.5062479999999563	F	F	F
1.4203730000000148	0.6205289999999453	3.5062479999999563	F	F	F
1.4203730000000148	4.4999990000000212	3.5062479999999563	F	F	F
4.7800929999999964	-1.3192070000000433	3.5062479999999563	F	F	F
4.7800929999999964	2.5602640000000059	3.5062479999999563	F	F	F
7.1047220603814205	-1.4732682628591700	11.1888351845091094	T	T	T
4.0410565551797060	0.4334238740189660	13.3089599040056541	T	T	T
6.9748469412251604	2.1281639189524997	13.3161069932753158	T	T	T

V302/CeO2 (111)

1.0		
13.4388805250000001	-7.7589412890000000	0.0000000000000000
0.0000000000000000	15.5178825770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.0000000000000000

Ce O V

48 98 3

Selective Dynamics

Cartesian

2.1621428755568228	-0.1226523630143901	10.6449878273998184	T	T	T
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5.5753229551568753	-2.0419016169950801	10.6162328892142011	T	T	T
5.6515478369996073	1.9150944166298824	10.3753094351162343	T	T	T
2.3247584776012551	7.9625212801957961	10.6169146519179094	T	T	T
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5.5870594166444603	5.9509984621194949	10.6630462687961529	T	T	T
5.6019048311541857	9.7495974453462502	10.6614925837889949	T	T	T

8.9968778545126931	-4.0256687171707730	10.5429401891785197	T T T
9.0498825838224342	0.0170080315787278	10.6212191431472807	T T T
12.1335915742395120	-5.7937312968737409	10.6040187711245046	T T T
12.1254731473301529	-1.9203555335684719	10.6654378112727422	T T T
9.0758989442158118	3.9069479922469892	10.6159442751545203	T T T
9.0373550418703275	7.9098426867470648	10.5340861550360128	T T T
12.3513955914615536	1.9436785983745937	10.6479130917843019	T T T
12.3306245745405327	5.7836322296135494	10.7174289343045839	T T T
13.4385738936874954	-7.7474431679962166	7.4483180144937933	T T T
13.4299187851523456	-3.8691695126250214	7.3979348417295885	T T T
3.3598508919943875	-1.9352339415605155	7.4372557579524532	T T T
3.3481671715156414	1.9205050851049501	7.4013522246866179	T T T
0.0120387803147993	7.7500157165278640	7.5036806807482037	T T T
0.0024155514624780	11.6458378410273635	7.4566712994660556	T T T
3.3517721155452396	5.8190036025289942	7.4660602012318407	T T T
3.3640145724144004	9.7068417595042060	7.4301419469391208	T T T
6.7219372416864989	-3.8799210753880962	7.4213710197161049	T T T
6.7417726465348871	-0.0262670092615589	7.4182275152381436	T T T
10.0807139887879735	-5.8076548164112296	7.3425077586377441	T T T
10.0689276007003539	-1.9374665892157057	7.4153530200157540	T T T
6.7243994307666135	3.9114802202686820	7.4331973885863896	T T T
6.7163770773264346	7.7579336662336429	7.4413129769279056	T T T
10.0747847689595496	1.9379817771263861	7.4436518317158225	T T T
10.0822014796225030	5.8296662117171749	7.4430962091279680	T T T
1.1199067103999885	1.9397353220999816	4.2969520308999307	F F F
1.1199067103999885	5.8192059664000411	4.2969520308999307	F F F
4.4796268417000240	-0.0000000001999654	4.2969520308999307	F F F
4.4796268417000240	3.8794706440999835	4.2969520308999307	F F F
1.1199067103999885	9.6986766105999838	4.2969520308999307	F F F
1.1199067103999885	13.5781472549000419	4.2969520308999307	F F F
4.4796268417000240	7.7589412883000346	4.2969520308999307	F F F
4.4796268417000240	11.6384119325999826	4.2969520308999307	F F F
7.8393469728999881	-1.9397353225000247	4.2969520308999307	F F F
7.8393469728999881	1.9397353219000415	4.2969520308999307	F F F
11.1990671042000240	-3.8794706446999649	4.2969520308999307	F F F
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7.8393469728999881	5.8192059660999833	4.2969520308999307	F F F
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11.1990671042000240	3.8794706438000350	4.2969520308999307	F F F
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2.2846442460398610	1.8392610489261172	12.4949231891378805	T T T
4.8553686677772276	0.4415538543951860	12.6568175538208578	T T T
4.8107913194814742	3.2922385972188919	12.6448633524594829	T T T
1.0905286157405349	9.8482485165672813	11.4416218146351714	T T T
1.1755510508908737	13.4428624280599536	11.4678371909331691	T T T
4.6345364140072567	7.9984627065227256	11.4724898028779450	T T T
4.4790377633787219	11.5425861121345292	11.4515571874069799	T T T
7.3726283121045058	-1.0302188288504555	12.4485466869637325	T T T
7.3191915081878935	1.9117922009655874	12.5850042851442510	T T T
10.9788049240479193	-4.0501036807288608	11.4955472443103552	T T T
11.2364706969263040	0.1292935864504141	11.4823299846684748	T T T
7.2993349388348028	4.8737637185393412	12.4652740034136791	T T T
7.9237753908057140	9.7223907443359678	11.4228025536726605	T T T
11.2883539496930894	3.7558564832018417	11.4488003418373765	T T T
11.0709131479206171	7.9663891405036953	11.4775535572326248	T T T
0.0323003877248607	0.2598321159979692	9.9958037441899030	T T T
0.0602794607104017	3.7977329436316469	10.3715262730719022	T T T
3.4334019563996794	-1.8581327860197556	9.8589587798505587	T T T
3.4422484633314490	1.8521498374146905	9.8600451453332756	T T T
0.0598633427220924	7.6300622672482348	9.8989301324862247	T T T
0.0190859008301455	11.6196024822000279	9.7109556058623703	T T T
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3.3997258561438009	9.7958337908685369	9.7421929802309517	T T T
6.8532032257570039	-3.7706310267738430	9.9074575281268871	T T T
6.7153480807919061	-0.0008911485338876	9.8596094075692520	T T T
10.0625080258839485	-5.8091843161088041	9.6893270775710167	T T T
9.8621079079527263	-1.9976167218650738	9.9577654795295540	T T T
6.7035088187794161	3.8489869005150665	9.8890721537855768	T T T
6.9053901254986414	7.6705242906888405	9.9125469816239740	T T T
9.9394999206032928	1.9526148024488306	9.8078524411346493	T T T
9.8797438407908214	5.9099280638924281	9.9571677226221649	T T T
2.1909982627331215	-0.0156044142600860	8.2080899292482190	T T T
2.1490239697801643	3.7850967848017065	8.2900183902931843	T T T
5.6186699862477969	-1.9681192329783801	8.1914715702739453	T T T
5.6277366619119649	1.9214793568652242	8.1062679001430666	T T T
2.2487695378296406	7.8158623553473676	8.2475016302952469	T T T
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5.6248074636177812	5.8553902442514278	8.2930837916561160	T T T
5.7062890121064553	9.7161441734700364	8.3340340279503238	T T T
8.9780517987476749	-3.8978132266807330	8.1984602277543548	T T T
8.9746712550032122	-0.0364716642597571	8.1874665677308229	T T T
12.3185977397272293	-5.7253266215273495	8.2768993767676822	T T T
12.2288977333753479	-2.0545153967503085	8.3206152655482715	T T T
8.9770878996253654	3.9310885497326140	8.1953249930009449	T T T
9.0008274120931677	7.7942604051212614	8.1919923452891563	T T T
12.2882165473308227	1.8755501103917771	8.2942937682297906	T T T
12.2728971897042687	5.9234446639757108	8.2937872922813245	T T T
1.0972663914422758	1.9351332362840972	6.6138626143586938	T T T
1.0129568758823515	5.8079092244272505	6.6561334302156592	T T T

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1.0871482348695281	13.5893250133670573	6.6360648768045154	T	T	T
4.5442105062970892	7.8492912075755266	6.6341224266802667	T	T	T
4.5017495767432347	11.6178367743532416	6.6324358243662882	T	T	T
7.8472484180286486	-1.9564318281035917	6.6160648801235649	T	T	T
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11.1988854963255857	-3.8797714032181356	6.5873096342185624	T	T	T
11.2186179255606202	-0.0306074554343949	6.6466705899151268	T	T	T
7.8357810211401269	5.8393579715755868	6.6324334413877519	T	T	T
7.8383013714596350	9.7048176781606692	6.6079907377106126	T	T	T
11.2197105708172771	3.8896549212866525	6.6569813831964559	T	T	T
11.2211889098874131	7.7919350103161351	6.6177223115802617	T	T	T
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3.3597201313000356	13.5781472546999407	5.0875064649998913	F	F	F
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0.0000000000000000	7.7589412885000000	5.0875064649998913	F	F	F
0.0000000000000000	11.6384119327000519	5.0875064649998913	F	F	F
3.3597201313000356	5.8192059662999487	5.0875064649998913	F	F	F
3.3597201313000356	9.6986766104999997	5.0875064649998913	F	F	F
6.7194402625000000	-3.8794706445000000	5.0875064649998913	F	F	F
6.7194402625000000	-0.0000000002999490	5.0875064649998913	F	F	F
10.0791603936999632	9.6986766102000530	5.0875064649998913	F	F	F
10.0791603936999632	-1.9397353224999994	5.0875064649998913	F	F	F
6.7194402625000000	3.8794706440000000	5.0875064649998913	F	F	F
6.7194402625000000	7.7589412882000524	5.0875064649998913	F	F	F
10.0791603936999632	1.9397353218000584	5.0875064649998913	F	F	F
10.0791603936999632	5.8192059660000011	5.0875064649998913	F	F	F
2.2398134207999760	-0.0000000000999831	3.5062484074000504	F	F	F
2.2398134207999760	3.8794706441999653	3.5062484074000504	F	F	F
5.5995335521000111	-1.9397353224000409	3.5062484074000504	F	F	F
5.5995335521000111	1.9397353220000246	3.5062484074000504	F	F	F
2.2398134207999760	7.7589412884000168	3.5062484074000504	F	F	F
2.2398134207999760	11.6384119326999667	3.5062484074000504	F	F	F
5.5995335521000111	5.8192059661999664	3.5062484074000504	F	F	F
5.5995335521000111	9.6986766105000246	3.5062484074000504	F	F	F
8.9592536832999752	-3.8794706445999831	3.5062484074000504	F	F	F
8.9592536832999752	-0.0000000003000347	3.5062484074000504	F	F	F
12.3189738146000121	-5.8192059669000411	3.5062484074000504	F	F	F
12.3189738146000121	-1.9397353225999820	3.5062484074000504	F	F	F
8.9592536832999752	3.8794706439000164	3.5062484074000504	F	F	F
8.9592536832999752	7.7589412881999662	3.5062484074000504	F	F	F
12.3189738146000121	1.9397353216999660	3.5062484074000504	F	F	F
12.3189738146000121	5.8192059660000242	3.5062484074000504	F	F	F
3.6485434425971381	1.8745134143930766	14.8888555973179013	T	T	T
6.7488178468307272	0.1752233705923492	14.8438969525788949	T	T	T
6.6750506190885321	3.6249669093782466	14.8326041563188742	T	T	T
3.8023668540356326	1.8533726093987815	13.2878167196247077	T	T	T
6.6295872234488229	0.2864166626619911	13.2439765294787097	T	T	T
6.5829819530707248	3.5237147476514377	13.2301427122195427	T	T	T

V3O3/CeO2 (111)

1.0		
13.4388805250000001	-7.7589412890000000	0.0000000000000000
0.0000000000000000	15.5178825770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.0000000000000000

Ce O V

48 99 3

Selective Dynamics

Cartesian

2.1573403314899076	-0.0631441177314991	10.5979818297913120	T	T	T
2.1562021518082002	3.9551156564179375	10.5938572586435384	T	T	T
5.5622460895322572	-2.0516151909719627	10.5929752286588386	T	T	T
5.6246915661513643	1.9456797890234236	10.3474690764575019	T	T	T
2.2238062580699860	7.7991196050660623	10.5809812702717245	T	T	T
2.2254309313144707	11.6059441442074807	10.5834264587648939	T	T	T
5.5580757502330407	5.9444352027315022	10.5855506452312262	T	T	T
5.5771129000666644	9.7029372744982059	10.6400547938376171	T	T	T
8.9952382404585869	-3.9904924168616445	10.6369870215936064	T	T	T
9.1094211114114483	-0.0337183818148974	10.5893449316984078	T	T	T
12.1431032852809615	-5.8186806412093892	10.5508380913074493	T	T	T
12.3392631864655264	-1.9297464364466252	10.6370452397986739	T	T	T
9.1070946244183091	3.9185800386269198	10.5901192090239800	T	T	T
8.9901239539507891	7.8656499370117494	10.6432577431204152	T	T	T
12.3803910376535207	1.9417998111085133	10.5893157914040383	T	T	T
12.3399756856886889	5.8122532109703844	10.6375434102202409	T	T	T
13.4348528080903081	-7.7471295824610165	7.4320868515694993	T	T	T
13.4339308678045448	-3.8894557597339898	7.4319685306871559	T	T	T
3.3668348304880191	-1.9234456469518308	7.4281698075596889	T	T	T
3.3375397304945889	1.9415650833598979	7.4158387186306429	T	T	T
0.0025321123618970	7.7525502193961024	7.4338536340009664	T	T	T
0.0030043581004244	11.6477392388351735	7.4343163572664572	T	T	T
3.3655632969117919	5.8075614824255091	7.4261234216813214	T	T	T
3.3731697281260122	9.7011084051874636	7.4326373697534240	T	T	T
6.7256997143750912	-3.8769581426374327	7.4437666652379466	T	T	T
6.7402525073879449	-0.0244377155587432	7.4168820806807387	T	T	T

10.0543843310747452	9.6978348056210919	7.3847038843488182	T	T	T
10.0785314565414374	-1.9588789880663899	7.4458225253069088	T	T	T
6.7403777801716345	3.9067505978253636	7.4157004717455663	T	T	T
6.7263471555415206	7.7604976921272568	7.4426248476494044	T	T	T
10.0783558683029320	1.9407097909005859	7.4289665278033699	T	T	T
10.0785787613748372	5.8395153874436811	7.4453503581225426	T	T	T
1.1199067103999885	1.9397353220999816	4.2969520308999307	F	F	F
1.1199067103999885	5.8192059664000411	4.2969520308999307	F	F	F
4.4796268417000240	-0.0000000001999654	4.2969520308999307	F	F	F
4.4796268417000240	3.8794706440999835	4.2969520308999307	F	F	F
1.1199067103999885	9.6986766105999838	4.2969520308999307	F	F	F
1.1199067103999885	13.5781472549000419	4.2969520308999307	F	F	F
4.4796268417000240	7.7589412883000346	4.2969520308999307	F	F	F
4.4796268417000240	11.6384119325999826	4.2969520308999307	F	F	F
7.8393469728999881	-1.9397353225000247	4.2969520308999307	F	F	F
7.8393469728999881	1.9397353219000415	4.2969520308999307	F	F	F
11.1990671042000240	-3.8794706446999649	4.2969520308999307	F	F	F
11.1990671042000240	-0.0000000004000160	4.2969520308999307	F	F	F
7.8393469728999881	5.8192059660999833	4.2969520308999307	F	F	F
7.8393469728999881	9.6986766104000424	4.2969520308999307	F	F	F
11.1990671042000240	3.8794706438000350	4.2969520308999307	F	F	F
11.1990671042000240	7.7589412880999831	4.2969520308999307	F	F	F
2.2608062263155002	1.9723305805073286	12.4478935128604089	T	T	T
1.0187992588096337	5.9255168256016928	11.3876902462217728	T	T	T
4.8382232061253436	0.5521080974324541	12.6124997423456371	T	T	T
4.8300719870429392	3.4194630174167919	12.5670272069458253	T	T	T
1.1215418773521317	9.7021443422868945	11.3855667816550792	T	T	T
1.0203044414675613	13.4784694148275079	11.3888662312190778	T	T	T
4.3776333434481316	7.8876606053540002	11.4039754148379089	T	T	T
4.3783225535625272	11.5190856710741940	11.4070724822638017	T	T	T
7.3624582380481796	-0.9580317680544721	12.4357882701482616	T	T	T
7.3120392537460637	1.9902943914815596	12.5700869313459123	T	T	T
11.3128627081011999	-3.9289494254639856	11.4478814892527971	T	T	T
11.3830357381437501	-0.0210211909242037	11.4137116662310056	T	T	T
7.35848773180565182	4.9433953961041279	12.4038160854223349	T	T	T
7.6576224052828197	9.6996444118024527	11.4830318576195189	T	T	T
11.3828113052054611	3.8981926392360320	11.4133087321479199	T	T	T
11.3127835786150666	7.8026530293615615	11.4480198516110310	T	T	T
0.0434573512455880	0.1874369093980469	9.8689126637241884	T	T	T
0.0409902679693158	3.6958622729767923	9.8660600284892528	T	T	T
3.3988652959016949	-1.8496672550753537	9.8908711256076174	T	T	T
3.3980064432266550	1.9427357041540312	9.8506173664616004	T	T	T
0.0314184498901676	7.8033859155640952	9.7259497228809231	T	T	T
0.0322584203771593	11.5982741837210526	9.7262295256584004	T	T	T
3.3925424713375709	5.7437065475952620	9.8811206958017781	T	T	T
3.2985488939441061	9.7021722435594580	9.7228029110244698	T	T	T
6.7533770357221190	-3.7860410856691784	9.8423272876770955	T	T	T
6.7279919102075381	0.0199836469656964	9.8519282176102578	T	T	T
10.0690050140923830	9.6959833571390774	9.7806552621470093	T	T	T
10.0272064958209306	-1.9626380890171569	9.8779301934732455	T	T	T
6.7291352509075706	3.8675071351864325	9.8516594473429144	T	T	T
6.7501686246388832	7.6799285781032118	9.8341790809010909	T	T	T
10.0222520359200207	1.9407115607720327	9.8892274282127879	T	T	T
10.0260676023138906	5.8405367310220448	9.8769684123243877	T	T	T
2.2251361617929026	-0.0047997896154515	8.1909556220419013	T	T	T
2.2250356024696374	3.8875131972349797	8.1873723267673810	T	T	T
5.5898431859242059	-1.9355053999182099	8.1854841939937906	T	T	T
5.6043518339694121	1.9421464371212105	8.0785128199884610	T	T	T
2.27157061797113315	7.7046857744842203	8.2412380880016283	T	T	T
2.2746396330628986	11.7011613486428558	8.2451771519980124	T	T	T
5.5902526250512095	5.8185993303200956	8.1808154248545115	T	T	T
5.6324432612304012	9.7041339891743661	8.2896480865963955	T	T	T
8.9689650868633439	-3.9002297176740344	8.1812941733001736	T	T	T
8.9869898906951242	-0.0109826823054862	8.1910849563163382	T	T	T
12.2592055798957755	-5.8195308628865883	8.2047412939421829	T	T	T
12.3237217101839178	-1.9951939978592064	8.3142936443712419	T	T	T
8.9869614579319670	3.8885908945043886	8.1920179025685815	T	T	T
8.9695985804414420	7.777551333680277	8.1810670501512188	T	T	T
12.2671290906656036	1.9409845343113767	8.2435535674270888	T	T	T
12.3239696151158338	5.8779956990729971	8.3155451898251886	T	T	T
1.0995773785599010	1.9401972418235736	6.6311045285619725	T	T	T
1.0942415811856110	5.8201023045360660	6.6279543634698079	T	T	T
4.4706290993426121	-0.0051816807428113	6.6179458347666218	T	T	T
4.4702599166937746	3.8864936169902635	6.6170478866697993	T	T	T
1.1223379768607720	9.7016059728926329	6.6627411981131193	T	T	T
1.0948858787081759	13.5795220341233538	6.6284992539053258	T	T	T
4.4869275585608035	7.7795753145734459	6.6308073480228735	T	T	T
4.4868097778137530	11.6220443593905465	6.6302097450177531	T	T	T
7.8461968144641769	-1.9442051435712973	6.6296060811482196	T	T	T
7.8624077347215042	1.9399974427938336	6.6237142590753839	T	T	T
11.2111273575291364	-3.8650571594640568	6.6151813971356495	T	T	T
11.2225945324999987	-0.0260640304217663	6.6372204408963151	T	T	T
7.8476532799161980	5.8242026277229285	6.6288524981543127	T	T	T
11.2229832606057318	9.6989422035054371	6.6136941768866038	T	T	T
11.2116526728447283	3.9070535301509697	6.6376702875551725	T	T	T
0.0000000000000000	7.7444870059253264	6.6145444029945661	T	T	T
0.0000000000000000	0.0000000000000000	5.0875064649998913	F	F	F
0.0000000000000000	3.8794706442000511	5.0875064649998913	F	F	F
3.3597201313000356	13.5781472546999407	5.0875064649998913	F	F	F

3.3597201313000356	1.9397353220000004	5.0875064649998913	F F F
0.0000000000000000	7.7589412885000000	5.0875064649998913	F F F
0.0000000000000000	11.6384119327000519	5.0875064649998913	F F F
3.3597201313000356	5.8192059662999487	5.0875064649998913	F F F
3.3597201313000356	9.6986766104999997	5.0875064649998913	F F F
6.7194402625000000	-3.8794706445000000	5.0875064649998913	F F F
6.7194402625000000	-0.0000000002999490	5.0875064649998913	F F F
10.0791603936999632	9.6986766102000530	5.0875064649998913	F F F
10.0791603936999632	-1.9397353224999994	5.0875064649998913	F F F
6.7194402625000000	3.8794706440000000	5.0875064649998913	F F F
6.7194402625000000	7.7589412882000524	5.0875064649998913	F F F
10.0791603936999632	1.9397353218000584	5.0875064649998913	F F F
10.0791603936999632	5.8192059660000011	5.0875064649998913	F F F
2.2398134207999760	-0.0000000000999831	3.5062484074000504	F F F
2.2398134207999760	3.8794706441999653	3.5062484074000504	F F F
5.5995335521000111	-1.9397353224000409	3.5062484074000504	F F F
5.5995335521000111	1.9397353220000246	3.5062484074000504	F F F
2.2398134207999760	7.7589412884000168	3.5062484074000504	F F F
2.2398134207999760	11.6384119326999667	3.5062484074000504	F F F
5.5995335521000111	5.8192059661999664	3.5062484074000504	F F F
5.5995335521000111	9.6986766105000246	3.5062484074000504	F F F
8.9592536832999752	-3.8794706445999831	3.5062484074000504	F F F
8.9592536832999752	-0.0000000003000347	3.5062484074000504	F F F
12.3189738146000121	-5.8192059669000411	3.5062484074000504	F F F
12.3189738146000121	-1.9397353225999820	3.5062484074000504	F F F
8.9592536832999752	3.8794706439000164	3.5062484074000504	F F F
8.9592536832999752	7.7589412881999662	3.5062484074000504	F F F
12.3189738146000121	1.9397353216999660	3.5062484074000504	F F F
12.3189738146000121	5.8192059660000242	3.5062484074000504	F F F
3.6589709745016870	2.0222890505791851	14.8158601510093817	T T T
6.7062814119567733	0.2580355391030560	14.8115800020082204	T T T
6.6723184136000375	3.7466329674684062	14.7785341873489813	T T T
3.7894527459879956	1.9906956424681628	13.2133159689696562	T T T
6.6075924979011758	0.3666948871943800	13.2106025759870267	T T T
6.5962321017670282	3.6188428133793509	13.1781585726908830	T T T

V3O4/CeO2 (111)

1.0		
13.4388805248000001	-7.7589412886000000	0.0000000000000000
0.0000000000000000	15.5178825772000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.0000000000000000

Ce O V

48 100 3

Selective Dynamics

Cartesian

2.0255099673078267	0.0098444359594143	10.5901156812959805	T T T
2.0651553227776716	3.8907743452063168	10.5700960635721000	T T T
5.4952904324668417	-2.1238743387766172	10.5620423125146239	T T T
5.6450125012000676	1.9962240055260230	10.6228677630576183	T T T
2.2266780907511028	7.7705465160117209	10.5536720861049425	T T T
2.2063514332621912	11.6008695417141130	10.5800828560311455	T T T
5.5337968497502885	5.9162808716103381	10.6209456641444877	T T T
5.5829551402139002	9.6616784235271886	10.6033268256845492	T T T
9.1147695134453226	3.9329144137091303	10.6088672510425113	T T T
9.0347505551744280	7.8568100770349796	10.5900811500619945	T T T
9.0635480731302511	-4.0221812029405779	10.5885344560211454	T T T
9.1205141313113991	0.0738073997163857	10.6354341746812882	T T T
12.3042594866782373	-5.7902742891224923	10.5983589123394140	T T T
12.3206671411251047	-1.9240198578759689	10.5979694157066575	T T T
12.3884274981535754	1.9401073936674589	10.5753217803800119	T T T
12.3289111941939389	5.7997588652228478	10.5997917195179703	T T T
13.4239319951116389	7.7660869915876312	7.4141708372519570	T T T
13.4219397893652506	-3.8843236781878590	7.4043272383148500	T T T
3.3509299400351811	-1.9254487720703011	7.4438186627848975	T T T
3.3615780278704923	1.9276570960129944	7.4660702740475235	T T T
13.4331403076359521	-0.0044169988272040	7.4274025995275004	T T T
0.0005301905902878	11.6384020686150524	7.4224141228278402	T T T
3.3675567974960332	5.7998774785921672	7.4434232751594829	T T T
3.3688538243960471	9.696556790258507	7.4272603679230533	T T T
6.7364527702026678	-3.8879535184073890	7.4407765776983625	T T T
6.7258613534010889	-0.0045465145742569	7.3780663190339641	T T T
10.0852391730229627	-5.8164450518402528	7.3926224745680909	T T T
10.0600346297642993	-1.9354618098724270	7.4585984926055486	T T T
6.7342218443797481	3.8858300269478425	7.4656417153736090	T T T
6.7292394195082545	7.7479921396299769	7.4432319157267086	T T T
10.0758199200240011	1.9506882120830413	7.4304277244991663	T T T
10.0772492342377511	5.8288369714229686	7.4322461398892381	T T T
1.1199067099519970	1.9397353229259637	4.2969520313999974	F F F
1.1199067099519970	5.8192059672259644	4.2969520313999974	F F F
4.4796268411519966	0.0000000007759637	4.2969520313999974	F F F
4.4796268411519966	3.8794706450759646	4.2969520313999974	F F F
1.1199067099519970	9.6986766115259648	4.2969520313999974	F F F
1.1199067099519970	13.5781472558259644	4.2969520313999974	F F F
4.4796268411519966	7.7589412893759642	4.2969520313999974	F F F
4.4796268411519966	11.6384119336759646	4.2969520313999974	F F F
7.8393469723519980	-1.9397353213740369	4.2969520313999974	F F F
7.8393469723519980	1.9397353229259640	4.2969520313999974	F F F
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Ce O V

48 101 3

Selective Dynamics

Cartesian

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2.2398134212480030 11.6384119321240362 3.5062484075999838 F F F
5.5995335524480030 5.8192059656740369 3.5062484075999838 F F F
5.5995335524480030 9.6986766099740365 3.5062484075999838 F F F
8.9592536836480026 -3.8794706450759642 3.5062484075999838 F F F
8.9592536836480026 -0.0000000007759642 3.5062484075999838 F F F
12.3189738148480021 -5.8192059672259635 3.5062484075999838 F F F
12.3189738148480021 -1.9397353229259640 3.5062484075999838 F F F
8.9592536836480026 3.8794706435240371 3.5062484075999838 F F F
8.9592536836480026 7.7589412878240367 3.5062484075999838 F F F
12.3189738148480021 1.9397353213740374 3.5062484075999838 F F F
12.3189738148480021 5.8192059656740369 3.5062484075999838 F F F
8.4241438134192261 3.8827908934304043 13.7120977125906762 T T T
3.6205683208007891 3.8282176355911526 14.5906868661909499 T T T
8.2260320366166813 1.1662279885230955 14.5910261716616674 T T T
5.8497644882687316 2.3720432665232885 13.5354697352118620 T T T

8.2869659996718834	6.5972699332649629	14.5981160058283876	T	T	T
5.8723231666102453	5.3568615726363138	13.7048994980359566	T	T	T
4.8284411554863524	3.8870997648632337	13.5250860316624966	T	T	T
7.6731948484573715	2.2440700953704065	13.5274906667280277	T	T	T
7.6761630822103823	5.5324388902552446	13.5556346887359496	T	T	T

V3O6/CeO2 (111)

1.0

13.4388810000000003 -7.7589410000000001 0.0000000000000000

0.0000000000000000 15.5178829999999994 0.0000000000000000

0.0000000000000000 0.0000000000000000 22.0000000000000000

Ce O V

48 102 3

Selective Dynamics

Cartesian

8.0827711943048790	4.4083506714103269	10.6226610176122982	T	T	T
1.4524618702345913	0.6257801011201055	10.5659299428452353	T	T	T
1.4173761119875741	4.5101018785287339	10.5771397529008127	T	T	T
4.7629573423375025	2.5368526284194108	10.5667178650808129	T	T	T
4.6132435067952464	6.4438369217713820	10.5540915436718894	T	T	T
1.4516254702809959	12.2607244610964639	10.5673689088693266	T	T	T
11.5812681734742338	2.4219280141073671	10.5564112165858663	T	T	T
1.4159633811797099	8.3773746706356089	10.5777048089945591	T	T	T
4.7621081490968660	10.3496072601623705	10.5665906866654264	T	T	T
11.5065641668028658	-1.3142769753981085	10.5776743869905019	T	T	T
11.5838972748921005	-5.0484795868911609	10.5514389654559597	T	T	T
11.6119551199729010	6.4454474437505116	10.6205878014794823	T	T	T
4.7797747479277062	-1.3160933296662909	10.5318472741536535	T	T	T
8.1251833875185699	-3.2264793148195485	10.5660138725264439	T	T	T
8.1253358361408132	0.5959213768741378	10.5672597700509208	T	T	T
8.0832896155483844	8.4822747753617449	10.6197580606680528	T	T	T
5.9038991430783101	4.5108528177222871	7.4425120092137966	T	T	T
5.9033443523331792	8.3726323551404125	7.4421279902677933	T	T	T
9.265678603408926	2.5703917897281787	7.4431597902805704	T	T	T
9.2596841017904161	6.4419995842900546	7.4976810152967808	T	T	T
5.9009516549764056	-3.2592033811230974	7.4199624792491630	T	T	T
5.9014524747640751	0.6247765059429500	7.4201458811373673	T	T	T
9.2653529210443217	-5.2036647182209821	7.4419091373942132	T	T	T
9.2669319347076495	-1.3168134568301477	7.4247565883078250	T	T	T
12.622333637913022	0.6170272086848501	7.4032286544349182	T	T	T
12.6094403452640869	4.5006853299974781	7.4426959885101338	T	T	T
2.5331058069276429	6.4416428103065702	7.4025835227964487	T	T	T
2.5359974868685224	10.3145856480666360	7.4248611031043064	T	T	T
12.6103862511667284	-7.1348870958876907	7.4419350852492805	T	T	T
12.6232784517023937	-3.2501819168173958	7.4020859107507793	T	T	T
2.5375277859908758	-1.3174635249654318	7.4200983217684993	T	T	T
2.5369165510408611	2.5685327680558294	7.4245702878749800	T	T	T
7.0199070000000008	6.4397350000000371	4.2969519999999628	F	F	F
7.0199070000000008	10.3192059999999763	4.2969519999999628	F	F	F
10.3796269999999833	4.5000000000000204	4.2969519999999628	F	F	F
10.3796269999999833	8.3794709999999597	4.2969519999999628	F	F	F
7.0199070000000008	-1.3192059999999763	4.2969519999999628	F	F	F
7.0199070000000008	2.5602639999999877	4.2969519999999628	F	F	F
10.3796269999999833	-3.2589419999999643	4.2969519999999628	F	F	F
10.3796269999999833	0.6205289999999719	4.2969519999999628	F	F	F
0.3004659999999645	10.3192060000000048	4.2969519999999628	F	F	F
0.3004659999999645	14.1986759999999688	4.2969519999999628	F	F	F
3.6601860000000412	8.3794699999999605	4.2969519999999628	F	F	F
3.6601860000000412	12.2589410000000090	4.2969519999999628	F	F	F
0.3004659999999645	2.5602640000000179	4.2969519999999628	F	F	F
0.3004659999999645	6.4397350000000064	4.2969519999999628	F	F	F
3.6601860000000412	0.6205289999999470	4.2969519999999628	F	F	F
3.6601860000000412	4.4999900000000221	4.2969519999999628	F	F	F
0.4917675247397874	14.2034061644844218	11.3363901684770596	T	T	T
12.5717517292365457	-7.0567454591402363	9.8345042361223367	T	T	T
10.8113262304669036	3.7883429622714448	14.6158538135170399	T	T	T
8.4051640849849427	4.9841500629832778	13.6320438266772701	T	T	T
10.5209305632573411	4.2622081167742873	11.9093507522584030	T	T	T
9.2589493223527839	6.4442366824440871	9.9959415633229636	T	T	T
0.3197065694300537	2.6378258669181442	11.3517283753058571	T	T	T
2.5459911023090687	2.5549722425413863	9.7619434530947302	T	T	T
6.9243036396445223	2.3986395869229713	11.3369978760191188	T	T	T
8.4024796191547022	7.9481654063041844	13.5915489956610713	T	T	T
7.0326701499146802	-1.3158478341067181	11.3390857327219852	T	T	T
5.8597873649626289	4.5876122655054381	9.8371808936450087	T	T	T
3.5889988017486552	4.5233421969749514	11.3527989382558392	T	T	T
3.6540598917306584	0.6349307896834886	11.3388828729533948	T	T	T
6.1630888070405137	6.4812439258857246	14.6034546434041275	T	T	T
6.7297864714744184	6.4445235629827149	11.9001070146694889	T	T	T
0.3189170685384634	10.2526531331193507	11.3536076524604379	T	T	T
3.5882353242132781	8.3636538834069380	11.3523417701789100	T	T	T
12.6387962568981163	0.5904071303834844	9.7492226791585139	T	T	T
12.5668245887832644	4.4267752890678826	9.8385195100003813	T	T	T
2.4986368274690229	6.4433156560177016	9.7478040786306579	T	T	T
2.5449965636546725	10.3313106324932846	9.7621941771319953	T	T	T
5.8587765477385263	8.3001766473234522	9.8364773977144360	T	T	T
0.3008082057741199	6.4451307826893087	11.3560730533623122	T	T	T
12.6414090917471409	-3.2173850289490113	9.7466131880129261	T	T	T

10.9692668556296997	6.4637405100440999	13.6168544892319812	T	T	T
5.8700214350502531	-3.2060954079211998	9.7307129345904677	T	T	T
10.4316890118563439	0.5725294531647611	11.3544310223251976	T	T	T
5.8713580445365574	0.5739368703189629	9.7309557047654387	T	T	T
9.3512224983623824	-5.1976346398766449	9.8344065157931926	T	T	T
9.2497373307416559	-1.3153000993817416	9.7620057451443660	T	T	T
9.3528924302720267	2.5703322989917909	9.8390486334455147	T	T	T
10.4340598775877762	-3.2017116930312839	11.3518062179011512	T	T	T
3.6528739161014641	12.2509278076631816	11.3399913981120548	T	T	T
2.5974083845085758	-1.3167874031690285	9.7309693078412334	T	T	T
6.9240740856087655	10.4897033156745962	11.3353470513290144	T	T	T
10.5282575015151814	8.6387081972517379	11.8870646326528338	T	T	T
10.8004806744118138	9.1565913013379223	14.5858319956338107	T	T	T
8.1370045375966100	4.4957277460328635	8.2220570618279218	T	T	T
8.1361657301180710	8.3885438761460556	8.2196607898664027	T	T	T
11.5194343117546296	2.5283345779406927	8.2170487903453591	T	T	T
11.5065864765971479	6.4423240330492053	8.2210529692011214	T	T	T
8.1470346016469595	-3.2815780927993972	8.2518451729217031	T	T	T
8.1482843364136830	0.6498236755460560	8.2532728018530612	T	T	T
11.5203091682607468	-5.1602501635682101	8.2155028307862921	T	T	T
11.4950223388619701	-1.3158203538138435	8.2161639736558634	T	T	T
1.4218969154458163	8.3859774007906083	8.2165532288584995	T	T	T
1.3921961455258796	12.2667306646807095	8.2529845236181156	T	T	T
4.7389936251035341	6.4422545331706047	8.2160555253408543	T	T	T
4.7981551463310659	10.3006115832583269	8.2523109029514039	T	T	T
1.3948108406858999	0.6169734357464088	8.2517597313887769	T	T	T
1.4232598256577929	4.4982094578115657	8.2156259822965065	T	T	T
4.7800878747794693	-1.3166313461066155	8.1758223586729777	T	T	T
4.7991529944114637	2.5835829332448221	8.2532536763113935	T	T	T
7.0178686786398856	6.4405675093493242	6.6512309317302813	T	T	T
7.0194112791997352	10.3212588218497547	6.6298559618336297	T	T	T
10.3802755851768893	4.4999008157353009	6.6508799026077714	T	T	T
10.3808072783256300	8.3831754365985205	6.6506490693265867	T	T	T
7.0394253007326171	-1.3173019759035998	6.6335301029542117	T	T	T
7.0198347076313192	2.5617644494307026	6.6302123173718908	T	T	T
10.3728032889030288	-3.2545658680047569	6.6229874034311011	T	T	T
10.3726388495093325	0.6199979552036039	6.6231723384241823	T	T	T
0.3053926271444326	10.3250866282126079	6.6230440772127208	T	T	T
0.3007926689519603	14.2000239990096730	6.6301165283835966	T	T	T
3.6608429921628169	8.3878355328837166	6.6229110895019705	T	T	T
3.6497986253998533	12.2431471756020631	6.6338769947382916	T	T	T
0.3060344633620924	2.5572389590377886	6.6227938225138097	T	T	T
0.3005393489202729	6.4415625334216209	6.6136252876260402	T	T	T
3.6507378370888461	0.6389665567188101	6.6337989896971861	T	T	T
3.6617390178473634	4.4942839001210526	6.6230026608523431	T	T	T
5.90000000000000465	4.4999999999999805	5.0875060000000039	F	F	F
5.90000000000000465	8.3794709999999171	5.0875060000000039	F	F	F
9.25972000000000282	2.5602639999999912	5.0875060000000039	F	F	F
9.25972000000000282	6.4397349999999287	5.0875060000000039	F	F	F
5.90000000000000465	-3.2589420000000073	5.0875060000000039	F	F	F
5.90000000000000465	0.6205289999999315	5.0875060000000039	F	F	F
9.25972000000000282	-5.1986770000000222	5.0875060000000039	F	F	F
9.25972000000000282	-1.3192059999999737	5.0875060000000039	F	F	F
12.61944000000000098	0.6205289999999746	5.0875060000000039	F	F	F
12.61944000000000098	4.5000000000000231	5.0875060000000039	F	F	F
2.5402789999999911	6.4397349999999589	5.0875060000000039	F	F	F
2.5402789999999911	10.3192060000000065	5.0875060000000039	F	F	F
12.61944000000000098	-7.1384120000000388	5.0875060000000039	F	F	F
12.61944000000000098	-3.2589419999999638	5.0875060000000039	F	F	F
2.5402789999999911	-1.3192070000000273	5.0875060000000039	F	F	F
2.5402789999999911	2.5602640000000205	5.0875060000000039	F	F	F
8.1398129999999771	4.5000000000000373	3.5062479999999563	F	F	F
8.1398129999999771	8.3794709999999757	3.5062479999999563	F	F	F
11.49953400000000326	2.5602649999999469	3.5062479999999563	F	F	F
11.49953400000000326	6.4397350000000229	3.5062479999999563	F	F	F
8.1398129999999771	-3.2589419999999492	3.5062479999999563	F	F	F
8.1398129999999771	0.6205289999999897	3.5062479999999563	F	F	F
11.49953400000000326	-5.1986770000000391	3.5062479999999563	F	F	F
11.49953400000000326	-1.3192059999999906	3.5062479999999563	F	F	F
1.42037300000000148	8.3794699999999587	3.5062479999999563	F	F	F
1.42037300000000148	12.2589410000000054	3.5062479999999563	F	F	F
4.7800929999999964	6.4397350000000522	3.5062479999999563	F	F	F
4.7800929999999964	10.3192059999999906	3.5062479999999563	F	F	F
1.42037300000000148	0.6205289999999453	3.5062479999999563	F	F	F
1.42037300000000148	4.4999990000000212	3.5062479999999563	F	F	F
4.7800929999999964	-1.3192070000000433	3.5062479999999563	F	F	F
4.7800929999999964	2.5602640000000059	3.5062479999999563	F	F	F
7.3551926804723999	6.4634020480966852	13.5195416598616447	T	T	T
10.2112892709889138	4.8134909171363534	13.5275604224459496	T	T	T
10.2105976052488092	8.1115959848756702	13.5100202426145088	T	T	T

V408/CeO2 (111)

1.0

13.4388805248000001	-7.7589412886000000	0.0000000000000000
0.0000000000000000	15.5178825772000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.0000000000000000

Ce O V

48 104 4

Selective Dynamics
Cartesian

5.5658552934745043	-1.9922338762370051	10.5656506100653242	T T T
5.5993372460895277	9.7222056793503953	10.5538943951587463	T T T
8.9850549730650346	3.8982406579067419	10.5777135937711790	T T T
12.4307250760438759	1.9190833067820758	10.6589365369783717	T T T
12.3848404805038186	-2.0476738161669479	10.5972649308384206	T T T
5.4691345463935432	1.8543493083147338	10.5524455949973799	T T T
8.9531046362477387	-0.1764604452388960	10.5759686464245792	T T T
2.1323010362345425	3.8895468559855693	10.5909258567057325	T T T
12.3365517904673876	-5.8117869498495818	10.5716788881731105	T T T
5.5190470504554892	5.9087649689442614	10.6415711919801907	T T T
2.2247793061477865	-0.0001177402290786	10.5614759165631185	T T T
9.0144112747277596	7.8602326574414230	10.6594682667522704	T T T
12.4120211788547223	5.9487427643984736	10.5654807065419369	T T T
2.2572625817370051	11.6426468849561502	10.5520277707728152	T T T
8.9540224490146958	-3.9111041097746497	10.5739882305953081	T T T
2.2605685251799659	7.7910258313201854	10.5836338642426853	T T T
0.0015773563965804	0.0111053728036638	7.3991008929244879	T T T
13.4385898324581152	-3.8788091702809018	7.3992377561489713	T T T
3.3556085622219314	-1.9291829201890653	7.4190722283684112	T T T
3.3528310990281391	1.9542383175916711	7.4076287052208691	T T T
13.4342369022508858	-0.0032410598352568	7.4500237753769118	T T T
13.4223071952082336	3.8786951198088211	7.4487180587218447	T T T
3.3618103367781558	5.8138452601654400	7.4423697912153282	T T T
3.3617318402491074	9.6967304931093246	7.4240907809175249	T T T
6.7269851941535350	-3.8809318584696517	7.4194329572286160	T T T
6.7298265064833673	0.0112682048018198	7.4130221857034799	T T T
10.0825879891833914	9.6882305713755237	7.4288445448256688	T T T
10.0943287196966782	-1.9486085168637666	7.4167777204314902	T T T
6.7135201865747369	3.8753795803832625	7.4564452295406500	T T T
6.7334068491058749	7.7465900838904158	7.4631522545733011	T T T
10.0816191959751364	1.9262257758089865	7.4565863440000637	T T T
10.0789286935218385	5.8248709361608384	7.4533256203616665	T T T
1.1199067104000318	1.9397353222000040	4.2969520308999307	F F F
1.1199067104000318	5.8192059665000038	4.2969520308999307	F F F
4.4796268416000320	-0.0000000000000551	4.2969520308999307	F F F
4.4796268416000320	3.8794706442999445	4.2969520308999307	F F F
1.1199067104000318	9.6986766108000033	4.2969520308999307	F F F
1.1199067104000318	13.5781472551000046	4.2969520308999307	F F F
4.4796268416000320	7.7589412885999449	4.2969520308999307	F F F
4.4796268416000320	11.6384119328999454	4.2969520308999307	F F F
7.8393469728000316	-1.9397353222000038	4.2969520308999307	F F F
7.8393469728000316	1.9397353222000042	4.2969520308999307	F F F
11.1990671040000311	-3.8794706443000555	4.2969520308999307	F F F
11.1990671040000311	-0.0000000000000560	4.2969520308999307	F F F
7.8393469728000316	5.8192059665000029	4.2969520308999307	F F F
7.8393469728000316	9.6986766108000033	4.2969520308999307	F F F
11.1990671040000311	3.8794706442999445	4.2969520308999307	F F F
11.1990671040000311	7.7589412885999440	4.2969520308999307	F F F
2.2823758167795534	0.0355224414908604	8.2401407855225841	T T T
2.2188799983822221	3.8730362638066813	8.2116655141027088	T T T
5.6319669496785121	-1.8526664140111386	8.2794972433130205	T T T
5.5715889351497507	1.9128048439698131	8.1987123081284583	T T T
2.2407480825378423	7.7597681505867113	8.2606138420436732	T T T
2.2032401125152634	11.6386176083750215	8.2188735797587231	T T T
5.6135784672620144	5.7777588035274885	8.2359913361075705	T T T
5.6108025095829017	9.6835215248602591	8.2034092021550507	T T T
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Ce O V

48 106 5

Selective Dynamics

Cartesian

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11.2194400000061005	0.0000000000012941	5.0875059999960968	F	F	F
1.1402790000025496	1.9397349999935654	5.0875059999960968	F	F	F
1.1402790000025496	5.8192060000022128	5.0875059999960968	F	F	F
11.2194400000061005	3.8794709999943953	5.0875059999960968	F	F	F
11.2194400000061005	7.758940999996528	5.0875059999960968	F	F	F
1.1402790000025496	9.6986759999919236	5.0875059999960968	F	F	F
1.1402790000025496	13.5781470000004632	5.0875059999960968	F	F	F
6.7398129999970928	-0.00000000000032130	3.5062480000080853	F	F	F
6.7398129999970928	3.87947100000053256	3.5062480000080853	F	F	F
10.0995339999941880	-1.9397349999946463	3.5062480000080853	F	F	F
10.0995339999941880	1.93973500000106108	3.5062480000080853	F	F	F
6.7398129999970928	7.7589409999950369	3.5062480000080853	F	F	F
6.7398129999970928	-3.8794709999963142	3.5062480000080853	F	F	F
10.0995339999941880	5.81920600000037129	3.5062480000080853	F	F	F
10.0995339999941880	-5.81920600000031844	3.5062480000080853	F	F	F
0.0203730000040999	3.8794699999951088	3.5062480000080853	F	F	F
0.0203730000040999	7.75894100000036487	3.5062480000080853	F	F	F
3.3800930000006439	1.9397349999958668	3.5062480000080853	F	F	F
3.3800930000006439	5.81920600000045140	3.5062480000080853	F	F	F
0.0203730000040999	11.6384119999967499	3.5062480000080853	F	F	F
0.0203730000040999	-0.0000009999979921	3.5062480000080853	F	F	F
3.3800930000006439	9.6986759999942258	3.5062480000080853	F	F	F
3.3800930000006439	-1.9397359999972366	3.5062480000080853	F	F	F
8.2326820140959835	0.6838716101055953	13.3812387474245469	T	T	T
8.5277656444357763	7.3247365317887008	13.5837616680841364	T	T	T
5.5696428361432737	9.1381213822938161	13.4750314028842837	T	T	T
8.4197130292665285	3.9391615348314524	13.3602264673193272	T	T	T
2.6222093383503702	7.4929428294164211	13.3510053093143082	T	T	T

V6012/CeO2 (111)

1.0		
13.4388805250000001	-7.7589412890000000	0.0000000000000000
0.0000000000000000	15.5178825770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.0000000000000000

Ce O V

48 108 6

Selective Dynamics

Cartesian

5.5203136183340726	-2.0715036698501090	10.4953942706057983	T	T	T
5.6125204285262651	9.6843032651928684	10.5661766575030054	T	T	T
8.8969208228833878	3.7847134133202589	10.5130513657763451	T	T	T
12.4622247084230828	1.9290079055055296	10.6018039893198068	T	T	T
12.3812930499722267	-2.0586947704144203	10.5767727435591077	T	T	T
5.6655178033229232	1.9344797950711814	10.5990138099176185	T	T	T
8.9374790053475106	0.0673069240049236	10.5995927354310311	T	T	T
2.1175641263474678	3.8569556215548642	10.5730925242303115	T	T	T
12.2983877868948781	-5.8193056695165870	10.5874891217950218	T	T	T
5.5310897387737290	5.9209051577066489	10.6033064198728013	T	T	T
2.1194880035273149	0.0134923443738111	10.5797847131105094	T	T	T
9.0000404069832598	7.8663172048823462	10.5839092465751161	T	T	T
12.3335214966769744	5.8917981466453746	10.6771073100390463	T	T	T
2.2434807414436997	11.6458245488400784	10.5694465490187248	T	T	T
9.0229174678278543	-3.9268428766603147	10.6686556378061965	T	T	T
2.2601403447407873	7.7827296798059225	10.5777648219522025	T	T	T
13.4121524228800642	7.7577169299061071	7.4223075856670970	T	T	T

13.4352542470710290	-3.8950792891721600	7.3939657257759572	T	T	T
3.3480115962526749	-1.9299308537096653	7.4120308158654842	T	T	T
3.3603980152665782	1.9333211468684757	7.4494825539804141	T	T	T
0.0020371030298892	7.7523388297076963	7.4402001325010341	T	T	T
13.4273376700858478	3.8866444257142279	7.4538376909590989	T	T	T
3.3595794653691597	5.8123806751891802	7.4389019831980123	T	T	T
3.3681215511295615	9.7065464074297694	7.4214829494436527	T	T	T
6.7486592014563058	-3.8836986553137343	7.4233319423061550	T	T	T
6.7224995354165422	-0.0005630936563792	7.4257970235321533	T	T	T
10.0839589244230350	-5.8065864235845526	7.4179898255388972	T	T	T
10.0798445811146351	-1.9385558771643105	7.4644478330819730	T	T	T
6.7019759331165423	3.8844456295283494	7.4270941826531214	T	T	T
6.7268129464685282	7.7463490706897726	7.4337800302384878	T	T	T
10.0964166876340737	1.9283210186182576	7.4302101957786864	T	T	T
10.0795192807265455	5.8155244731298357	7.4533491218645906	T	T	T
1.1199067104122100	1.9397353221375813	4.2969520308960236	F	F	F
1.1199067104122100	5.8192059663875817	4.2969520308960236	F	F	F
4.4796268416622098	-0.0000000001589471	4.2969520308960236	F	F	F
4.4796268416622098	3.8794706440910529	4.2969520308960236	F	F	F
1.1199067104122100	9.6986766106375839	4.2969520308960236	F	F	F
1.1199067104122100	13.5781472548875826	4.2969520308960236	F	F	F
4.4796268416622098	7.7589412883410516	4.2969520308960236	F	F	F
4.4796268416622098	11.6384119325910511	4.2969520308960236	F	F	F
7.8393469729122103	-1.9397353224710256	4.2969520308960236	F	F	F
7.8393469729122103	1.9397353218875812	4.2969520308960236	F	F	F
11.1990671041622107	-3.8794706446589475	4.2969520308960236	F	F	F
11.1990671041622107	-0.0000000004089475	4.2969520308960236	F	F	F
7.8393469729122103	5.8192059661375826	4.2969520308960236	F	F	F
7.8393469729122103	9.6986766103875812	4.2969520308960236	F	F	F
11.1990671041622107	3.8794706438410511	4.2969520308960236	F	F	F
11.1990671041622107	7.7589412880910515	4.2969520308960236	F	F	F
2.2209826841439306	0.0169918002124421	8.2475734699137284	T	T	T
2.2422372096119632	3.8395213025090387	8.2417819829052927	T	T	T
5.5869451120541278	-1.9695106883683251	8.1951957342557922	T	T	T
5.6298247726442909	1.9301831018941957	8.2176675655085063	T	T	T
2.2388907529154660	7.7456623533094291	8.2654801743059636	T	T	T
2.2433424330412604	11.6917918024121370	8.2527310159263312	T	T	T
5.5647857085825940	5.8347650757503926	8.1725018783903352	T	T	T
5.6505106841923318	9.6967086063747665	8.2523912739487919	T	T	T
8.9741846191346504	-3.8463665156957836	8.2093803891281372	T	T	T
8.9240365166444597	0.0296238576170618	8.2158806069229087	T	T	T
12.3126051223709805	-5.8219742475694769	8.2093232771519489	T	T	T
12.3222638782518370	-1.9719868299121757	8.2302733266889039	T	T	T
8.9365162773019868	3.8368614742508900	8.2204021368875519	T	T	T
8.9996999632559938	7.7468735458333740	8.2474839490375320	T	T	T
12.3594041125441283	1.9237633820933109	8.1817220719853978	T	T	T
12.2652734260516478	5.8362973191880565	8.2362567137206444	T	T	T
1.1239686288469855	1.9326687472374111	6.6217291647244698	T	T	T
1.1271245910748560	5.8128713836670336	6.6343707765798783	T	T	T
4.4713413381218761	0.0011747818242598	6.6397150917744927	T	T	T
4.4685072317890757	3.8625196098331189	6.6363514949105511	T	T	T
1.1460656190231904	9.7039470751675942	6.6400825672147050	T	T	T
1.10919622205167893	13.5861950872307045	6.6357784527339341	T	T	T
4.4717454527054068	7.7779199048369794	6.6330598596529757	T	T	T
4.4786118086739410	11.6294438835693352	6.6289222199963946	T	T	T
7.8365422318818148	-1.9297133284128281	6.6324388923479409	T	T	T
7.8356277163334731	1.9396802310631838	6.6155128055151602	T	T	T
11.2038986982976372	-3.8757192169287134	6.6189367743386054	T	T	T
11.1979128887872488	-0.0147553456913450	6.6451571295765106	T	T	T
7.8485571201183042	5.8152200556895348	6.6437035090078309	T	T	T
7.8492734141774294	9.6914563523882400	6.6310158033447308	T	T	T
11.1915662040748458	3.8792433787919540	6.6440542072881135	T	T	T
11.1928896480705138	7.7582729058307338	6.6182230505186626	T	T	T
0.0000000000000000	0.0000000000000000	5.0875064650080200	F	F	F
0.0000000000000000	3.8794706442500000	5.0875064650080200	F	F	F
3.3597201312500000	13.5781472547034703	5.0875064650080200	F	F	F
3.3597201312500000	1.9397353220465303	5.0875064650080200	F	F	F
0.0000000000000000	7.7589412885000000	5.0875064650080200	F	F	F
0.0000000000000000	11.6384119327499995	5.0875064650080200	F	F	F
3.3597201312500000	5.8192059662965301	5.0875064650080200	F	F	F
3.3597201312500000	9.6986766105465296	5.0875064650080200	F	F	F
6.7194402625000000	-3.8794706445000000	5.0875064650080200	F	F	F
6.7194402625000000	-0.0000000002500000	5.0875064650080200	F	F	F
10.0791603937499996	9.6986766102034707	5.0875064650080200	F	F	F
10.0791603937499996	-1.9397353225465306	5.0875064650080200	F	F	F
6.7194402625000000	3.8794706440000000	5.0875064650080200	F	F	F
6.7194402625000000	7.7589412882500000	5.0875064650080200	F	F	F
10.0791603937499996	1.9397353217965296	5.0875064650080200	F	F	F
10.0791603937499996	5.8192059660465292	5.0875064650080200	F	F	F
2.2398134208377902	-0.0000000000910527	3.5062484074019271	F	F	F
2.2398134208377902	3.8794706441589470	3.5062484074019271	F	F	F
5.5995335520877907	-1.9397353223875815	3.5062484074019271	F	F	F
5.5995335520877907	1.9397353219710252	3.5062484074019271	F	F	F
2.2398134208377902	7.7589412884089475	3.5062484074019271	F	F	F
2.2398134208377902	11.6384119326589470	3.5062484074019271	F	F	F
5.5995335520877907	5.8192059662210252	3.5062484074019271	F	F	F
5.5995335520877907	9.6986766104710238	3.5062484074019271	F	F	F
8.9592536833377903	-3.8794706445910521	3.5062484074019271	F	F	F
8.9592536833377903	-0.0000000003410525	3.5062484074019271	F	F	F

12.3189738145877890	-5.8192059668875817	3.5062484074019271	F F F
12.3189738145877890	-1.9397353226375813	3.5062484074019271	F F F
8.9592536833377903	3.8794706439089479	3.5062484074019271	F F F
8.9592536833377903	7.7589412881589483	3.5062484074019271	F F F
12.3189738145877890	1.9397353217210256	3.5062484074019271	F F F
12.3189738145877890	5.8192059659710242	3.5062484074019271	F F F
7.7851725599586885	9.6012185077507155	11.3770357776876860	T T T
6.7167213208939360	-3.8181596667868272	9.8097976677661336	T T T
10.0902710036151753	-5.8174217355350661	9.7516294244693995	T T T
4.4653103283851525	11.6528526351336765	11.3367253486734381	T T T
3.4165369304488911	-1.8405527338009282	9.7859799831484136	T T T
4.4038852906456736	7.9021273037376680	11.3584728852010777	T T T
3.3133515493427823	5.7434789294292612	9.8245677214429978	T T T
3.3869788052295795	9.7369726217547914	9.7100100076008324	T T T
6.7818702727978835	7.7245234173494604	9.7859943350035152	T T T
1.0757749059350272	1.9524205042798348	11.3800952848616159	T T T
1.0869201060256168	5.7125219843067381	11.3779739265650086	T T T
0.0116687393386073	3.8485250491491008	9.7285159365060832	T T T
13.4175025333424145	-0.0794910855146886	9.8293032892012597	T T T
1.3097227291220217	9.6868981941912082	11.3786485824749626	T T T
6.1432839702990680	4.7674021622900780	13.9068548940148311	T T T
8.1915929352969883	6.6261606467923162	14.4954227340830819	T T T
5.3418105440639581	1.9066977081301357	13.4719382056254311	T T T
3.5236854108919444	3.8554121449648879	14.4787538987917497	T T T
11.3273332531707673	-0.0586500892863713	11.9023929584561277	T T T
6.7232141041947076	3.9681357333990741	9.8386118878400612	T T T
11.6083959832336490	-0.8242612015671691	14.5274747656596706	T T T
11.1876159349484183	3.8384547847167809	11.8626307502768604	T T T
11.0942616420220599	1.9069637220577178	13.9916192086274371	T T T
11.6992286648442345	4.6334866169345883	14.4204492521039249	T T T
7.8302699955513884	5.8962587119949488	11.8781056745469638	T T T
9.0368236570538087	4.0636236506034145	13.6312066411943480	T T T
11.3703644016778647	-3.9123562614537057	11.4041922185604623	T T T
4.4058741331127838	-0.1537450323463583	11.8568313230641778	T T T
7.684238275858008	-2.0053866824536817	11.8651362451720210	T T T
3.3607168261595142	1.9235630416227247	9.8932819575696360	T T T
6.6297969828931445	-0.1470404527794091	9.9034650565155360	T T T
10.1543610672585345	-1.8610142760697554	9.8920684018741163	T T T
10.1557063009077986	1.9943670092928851	9.8314173938417468	T T T
4.3398046141974103	3.9266232162959396	11.8530864049299058	T T T
9.0343007918238118	-0.2048130273503377	13.4793445182397456	T T T
11.1128801702220574	7.8916020332083461	11.3933151092015752	T T T
1.2560014140735276	13.6404712202912819	11.3751062670609446	T T T
9.9296310372642669	5.7264436051555396	9.9233892484902029	T T T
0.0198207176416112	11.6547764510559073	9.8200374722399282	T T T
13.4373525877368681	-7.7139428625657080	9.7853412672943723	T T T
3.4952626972817731	-0.0228086888431123	14.4453089840736322	T T T
8.2607700656701066	-2.7671364715759217	14.4272361466197285	T T T
7.9084642220811388	2.0704131709759164	11.3818933410411134	T T T
6.1594868493523602	-0.9001658037245237	14.0492866884474701	T T T
7.8046988352989244	5.3814499008342764	13.5515659565827509	T T T
4.7986274865505454	3.6380106939652426	13.5218111043107996	T T T
10.8098340485824149	0.1813382972695772	13.5582066653863613	T T T
10.7842321209407253	3.6278891794601309	13.5549266085889908	T T T
4.8069407520506360	0.1723694964399067	13.5337789494007072	T T T
7.7775784132854771	-1.5108313995659155	13.5424365932194792	T T T

V7014/CeO2 (111)

1.0		
13.4388810000000003	-7.7589410000000001	0.0000000000000000
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Ce O V

48 110 7

Selective Dynamics

Cartesian

7.3559053519380520	5.4267843998302432	10.6261867401731660	T T T
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7.3354682323550895	1.6951593049400628	10.5405334619901652	T T T
3.9199410371237335	-0.4255328397118374	10.4849239843884856	T T T
3.9033530773478788	7.5566389016441002	10.5555962520609494	T T T
4.0741857929743688	3.5444680328391791	10.5843794463966532	T T T
7.4074750528930942	-2.3228825317180792	10.7230358521363200	T T T
7.2863228583283890	9.4414368870577015	10.6341900390287396	T T T
0.5917232239027004	5.5202969868177307	10.6700388508695738	T T T
0.4936749913848617	1.6630565220956515	10.5865764833168186	T T T
10.8959525081963253	3.5627705904671139	10.4790891284718271	T T T
0.6489366757196003	13.3044531677670310	10.5683432616496145	T T T
0.6606867415956211	9.4086559226569282	10.5700597437197814	T T T
10.8026638568167535	-0.3518323568689903	10.6212126574347820	T T T
10.7388380970526729	7.4518441899185603	10.6203559562190453	T T T
10.8013883566831481	-4.0292686522691792	10.5748690996262678	T T T
5.1216629173587371	5.5135675153634534	7.4546385794411520	T T T
5.1256974103889830	9.3941546681963040	7.4318171875186181	T T T
8.4855872531641658	3.5848971718496401	7.4166815610993950	T T T
4.4691772837143553	7.4549178603566872	7.4806601154188703	T T T
5.1413545400919656	-2.2517565192079121	7.4298457315875917	T T T
5.1083259547919893	1.6308983675652797	7.4163119210290063	T T T

8.4874136231517276	-4.1827970171562017	7.4507648164793077	T T T
8.4904399878819863	-0.3162130043524396	7.4586011777248862	T T T
11.8420766718889858	1.6287561855515653	7.4071263298762906	T T T
11.8367493091735625	5.5449325455319993	7.4042664538437037	T T T
1.7631309796370724	7.4407888079372366	7.4352351500669016	T T T
1.7665561893628814	11.3462752801325077	7.4220413048580989	T T T
11.8016074338109913	-6.1117733622579804	7.4243621400953401	T T T
11.8549526370674361	-2.2426205100707088	7.4028928603230213	T T T
1.7400541253446344	-0.2866324625703275	7.4076726154951871	T T T
1.7511271403060524	3.5824238149079690	7.4602073078340680	T T T
6.2409659999961340	7.4557290000086915	4.2969520000080914	F F F
6.2409659999961340	11.3352000000017927	4.2969520000080914	F F F
9.6006860000060463	5.5159940000017276	4.2969520000080914	F F F
9.6006860000060463	9.3954639999914384	4.2969520000080914	F F F
6.2409659999961340	-0.3032129999930593	4.2969520000080914	F F F
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12.9604060000024948	3.5762579999992568	4.2969520000080914	F F F
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2.8812449999990388	5.5159930000069126	4.2969520000080914	F F F
5.0883829964932259	9.3949150780869672	9.7580002068544047	T T T
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7.2329518988278503	8.1754415502627857	14.2883523356578337	T T T
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9.7893229052432904	6.8120680803230833	14.2742984834513891	T T T
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7.4898508206378889	1.4525677993128010	13.4578208157487325	T T T
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6.7271808458547033	-1.1233430933042823	14.3565551700752252	T T T
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1.7584854929553082	11.3979082189597349	9.7243940491885166	T T T
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4.0288257480244827	11.3695640049860138	8.2365359530098345	T T T
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3.9683263395343342	-0.3308263770250273	8.1710412751852743	T T T
4.0323301155757889	3.5367211657057096	8.2038874720111767	T T T
6.2575281932442079	7.4460674465198480	6.6520064656234004	T T T

6.2529698207674356	11.3640640131717436	6.6311927928482524	T	T	T
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6.2640038212497728	-0.3114668650492924	6.6538406126041281	T	T	T
6.2452048922062042	3.5555473532945423	6.6125642956224349	T	T	T
9.5982752247041478	-2.2283970402059410	6.6201573625308461	T	T	T
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8.4807789999935821	-4.1826830000036619	5.0875059999960968	F	F	F
8.4807789999935821	-0.3032129999985154	5.0875059999960968	F	F	F
11.8404990000034953	1.63652300000031703	5.0875059999960968	F	F	F
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11.8404990000034953	-2.2429480000053683	5.0875059999960968	F	F	F
1.76133800000000394	-0.3032129999977139	5.0875059999960968	F	F	F
1.76133800000000394	3.5762579999953865	5.0875059999960968	F	F	F
7.3608719999945826	5.5159940000071472	3.5062480000080853	F	F	F
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10.7205930000050458	-4.1826830000091917	3.5062480000080853	F	F	F
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0.6414320000015896	9.3954640000054699	3.5062480000080853	F	F	F
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4.0011519999980392	7.4557290000063903	3.5062480000080853	F	F	F
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0.6414320000015896	1.6365220000038299	3.5062480000080853	F	F	F
0.6414320000015896	5.5159929999968211	3.5062480000080853	F	F	F
4.0011519999980392	-0.3032129999953606	3.5062480000080853	F	F	F
4.0011519999980392	3.5762579999977415	3.5062480000080853	F	F	F
6.2537239117574313	6.9426657748240501	13.4651991221218594	T	T	T
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9.2358882719878288	1.9594467341579493	13.5593876274964629	T	T	T
3.2849124024851251	1.8402792035851967	13.5471999579084468	T	T	T
3.3195900573249899	5.3044565769902299	13.5830257726730679	T	T	T
6.2367458811871082	0.1585387143042691	13.5117033679527339	T	T	T
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V8O16/CeO2 (111)

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Ce O V

48 112 8

Selective Dynamics

Cartesian

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4.7533987161418247	9.3754210289522213	10.6746460147916427	T	T	T
1.5799034644890086	-0.5425495338283857	10.5596427778671362	T	T	T
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11.6300281093503663	1.4570018110931224	10.5793030080803678	T	T	T
11.7006399951698477	5.4113511508752703	10.6001518574050309	T	T	T
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8.1163139518408887	7.3195860094962635	10.6021250231811770	T	T	T
8.1555431699933791	3.5534892901573345	10.5912230602026121	T	T	T
4.8323000451001521	-2.3718251541321416	10.5711483350458479	T	T	T
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2.6155592497069757	5.4116951445377186	7.4181637652947554	T	T	T
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2.6147262779311773	9.2778907969720166	7.4251038796363549	T	T	T
2.6116655904236188	13.1608926202110386	7.3912378453950822	T	T	T
5.9664510641977939	7.3748448366810164	7.4188149386601925	T	T	T
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7.0903649999986156	1.5250160000063131	4.2969520000080914	F F F
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3.7306440000015195	11.2236929999993897	4.2969520000080914	F F F
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0.5517236706290771	13.1095467591707990	11.3741959658319765	T T T
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5.8500688004911519	7.1630326241315583	14.0901424083801601	T T T
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4.7969148591690560	9.1633961269327031	13.1640337728721661	T T T
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10.2753690674352036	5.6554956328077246	14.0806232419264852	T T T
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8.2017167349596658	-4.2577344944447857	8.2512513296919856	T T T
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11.5596079179144322	1.5035457912864736	8.2287732115451622	T T T
1.4555627743219826	3.5074916442365383	8.2079444392152716	T T T
1.4848097251607291	7.3220195840564060	8.2233978737450748	T T T
11.6255821229102949	5.4408986665326973	8.2034671863669484	T T T
11.5505849172632349	-6.2244296535491461	8.1993455622069344	T T T
1.4631838430356290	11.1905290551272589	8.2551832192693233	T T T
1.4873164412772706	-0.4170231438184060	8.2072017908174484	T T T
3.7223304918968347	3.4693351737953928	6.6387243591876022	T T T

3.7201465491461780	7.3329014511395005	6.6229013674747153	T	T	T
7.1111742507943987	1.4897914220881452	6.6634641813254927	T	T	T
7.1007253057262618	5.4146739941162592	6.6282126983933454	T	T	T
3.7088618433801219	11.2414835596423366	6.6141083513269958	T	T	T
3.7333101505270845	-0.4367672920619585	6.6252094849827152	T	T	T
7.1071777834089813	9.3049464069087406	6.6283605375044710	T	T	T
7.1079609943099120	-2.3430084744762558	6.6315337258899234	T	T	T
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0.3583879392100017	5.4076516775812342	6.6118853268993405	T	T	T
0.3659487814703135	9.2835919740504291	6.6220212652377191	T	T	T
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0.3811282304951718	13.1534716707252102	6.6186342345412150	T	T	T
0.3655765420353392	1.5369182225640934	6.6364613673290282	T	T	T
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5.9704579999996152	-0.4147190000052099	5.0875059999960968	F	F	F
5.9704579999996152	3.4647520000033287	5.0875059999960968	F	F	F
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9.3301779999960637	-2.3544540000043996	5.0875059999960968	F	F	F
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12.6898980000060728	-4.2941899999992614	5.0875059999960968	F	F	F
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9.3301779999960637	5.4044870000093956	5.0875059999960968	F	F	F
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4.8505510000006167	1.5250160000039590	3.5062480000080853	F	F	F
4.8505510000006167	5.4044869999970615	3.5062480000080853	F	F	F
8.2102709999970642	-0.4147189999952303	3.5062480000080853	F	F	F
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4.8505510000006167	9.2839580000057111	3.5062480000080853	F	F	F
4.8505510000006167	-2.3544550000046893	3.5062480000080853	F	F	F
8.2102709999970642	7.3442220000031302	3.5062480000080853	F	F	F
8.2102709999970642	-4.2941900000037689	3.5062480000080853	F	F	F
11.5699909999936086	-2.3544539999943641	3.5062480000080853	F	F	F
11.5699909999936086	1.52501600000107833	3.5062480000080853	F	F	F
1.4908310000040710	3.4647510000030950	3.5062480000080853	F	F	F
1.4908310000040710	7.3442219999961953	3.5062480000080853	F	F	F
11.5699909999936086	5.4044870000038845	3.5062480000080853	F	F	F
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1.4908310000040710	-0.4147200000054441	3.5062480000080853	F	F	F
9.9705230973756844	3.8961003357089954	13.6362646813347634	T	T	T
3.8271214180234372	3.6266161967174346	13.4508511722192328	T	T	T
6.9726402406278378	2.1480576882138021	13.5802516987480892	T	T	T
0.7339938845818594	1.9510851006501126	13.6907177456137834	T	T	T
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6.5864450543201638	8.7551877596046701	13.4990708500980450	T	T	T
9.9400886514087041	7.3042686817845368	13.4919523070623963	T	T	T

VO2-ML-a/CeO2 (111)

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13.4388805240000000	-7.7589412879999999	0.0000000000000000
0.0000000000000000	15.5178825780000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.0000000000000000

Ce O V

48 128 16

Selective Dynamics

Cartesian

2.3551327477810258	3.3034427826066093	10.6868819382997664	T	T	T
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5.7144881043840297	1.3753285902748611	10.6897904541471060	T	T	T
5.6927016582232230	5.2260178137498503	10.5332092871193712	T	T	T
0.1093275887708264	3.2873902929179843	7.4368833009187210	T	T	T
0.0840021248918446	7.1982378474806410	7.4286057417128859	T	T	T
3.4694779394563073	1.3820586521694262	7.4360135272647021	T	T	T
3.4447906331461597	5.2293042206834661	7.4288287652205378	T	T	T
1.2199067103000385	5.2397353222999641	4.2969520308999307	F	F	F
1.2199067103000385	1.3602646777999645	4.2969520308999307	F	F	F
4.5796268413000378	3.3000000002999643	4.2969520308999307	F	F	F
4.5796268413000378	7.1794706447999648	4.2969520308999307	F	F	F
2.3548363928931084	11.0621063674418263	10.6864843580459485	T	T	T
2.3330422008108602	-0.5471893628591400	10.5268415584719239	T	T	T
5.7142445897936831	9.1342291379417322	10.6902383991351986	T	T	T
5.6922547422480854	-2.5327455880407896	10.5328257667807144	T	T	T
0.1091999721273360	11.0461115686054061	7.4368469279885137	T	T	T
0.0839616753367742	14.9571839137449736	7.4285846969549336	T	T	T
3.4694295258090473	9.1408463530693425	7.4361239245466209	T	T	T
3.4446386879666155	12.9882357033590985	7.4287430733279720	T	T	T
1.2199067103000385	12.9986766112999650	4.2969520308999307	F	F	F
1.2199067103000385	9.1192059667999636	4.2969520308999307	F	F	F
4.5796268413000378	11.0589412892999661	4.2969520308999307	F	F	F

4.5796268413000378	-0.5794706442000352	4.2969520308999307	F F F
9.0744130584066802	3.3033715956361069	10.6863867387898086	T T T
9.0524102926977612	7.2115237741198861	10.5275604290925919	T T T
12.4335777931891727	1.3745741167717034	10.6898400906871132	T T T
12.4119163288236756	5.2255718981591155	10.5324821583933073	T T T
6.8286802344119275	3.2873445329565447	7.4370191456743928	T T T
6.8034986730198401	7.1983632354213487	7.4288818107236789	T T T
10.1888437419237547	1.3817232306824305	7.4361835307405331	T T T
10.1641274121802656	5.2291472557967422	7.4288573938741171	T T T
7.9393469723000392	5.2397353222999303	4.2969520308999307	F F F
7.9393469723000392	1.3602646777999299	4.2969520308999307	F F F
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11.2990671033000396	7.1794706447999301	4.2969520308999307	F F F
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9.0526506527933464	-0.5473906198178415	10.5272374026661186	T T T
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12.4121260523164985	-2.5334266907322389	10.5327017419738578	T T T
6.8285604879748147	11.0462098979072625	7.4370567694052516	T T T
6.8035324093633482	-0.5605928178576183	7.4287188568829938	T T T
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10.1642071298550629	-2.5297514675303621	7.4287473872557470	T T T
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4.5577968134861777	3.3658574075084560	12.0507531211860250	T T T
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0.1186949837395016	3.2666670751091451	9.9488222878867987	T T T
0.0671417635517973	7.2239170232054128	9.8525809688808010	T T T
3.4820063852186434	1.4107495386822104	9.9471649085134697	T T T
3.4305132959624651	5.2123829338033563	9.8470266071102870	T T T
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2.3437481132195774	7.2075465320867389	8.1896927669677719	T T T
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5.7057917233124504	5.2229025732089163	8.1916263442612411	T T T
1.2239492382337613	5.2412378657324448	6.6371071139428679	T T T
1.2105777081800335	1.3640356278838901	6.6270437490085392	T T T
4.5702211809736113	3.3029929617680280	6.6276291945744452	T T T
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3.0682772427136524	0.4771353068683630	13.7036418915011602	T T T
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4.5289493566421299	2.79364779141165256	14.8373459482871581	T T T
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1.1493320042159190	1.9117867200361454	14.8278874534744904	T T T
1.1511098111426898	6.6375157487847902	14.3121166645143560	T T T
1.1663571353782625	13.1958866124912380	11.7816921750365928	T T T
1.2014547017373065	9.0877186640954033	12.0407360065482933	T T T
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4.5085147419522453	-0.7602779803436481	11.7886290583528144	T T T
0.1180503623743071	11.0255827834489750	9.9490870373879670	T T T
0.0672063403485872	14.9829378145065863	9.8526414937495179	T T T
3.4815682098547165	9.1694418682334184	9.9467421326165084	T T T
3.4301896865033008	12.9712230309942314	9.8464751240491939	T T T
2.3243607479851658	11.0405246613821522	8.2205621932261081	T T T
2.3437679153424695	-0.5511813640179355	8.1896138656840929	T T T
5.6857217403881339	9.1474848877050405	8.2202330719645023	T T T
5.7058940078374256	-2.5357377700358130	8.1914667472059470	T T T
1.2239553605928724	13.0002169187360614	6.6372107839529315	T T T
1.2106191375945476	9.1228421940331987	6.6269354441793205	T T T
4.5701333585731865	11.0619756832315570	6.6277988076395413	T T T
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4.529190358411430	10.5530555521704699	14.8377568949738325	T T T
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9.0592536826999606	3.3000000001999705	3.5062484074000504	F	F	F
9.0592536826999606	7.1794706446999719	3.5062484074000504	F	F	F
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12.4189738136999601	5.2397353226999721	3.5062484074000504	F	F	F
9.7890037445930691	0.4769785297956988	13.7043636552296491	T	T	T
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7.8858996466591238	-2.3218977906239049	11.7814896483052358	T	T	T
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11.2763906000091652	-4.3933021902743112	12.0499705559940509	T	T	T
12.2285526549645489	-0.7620716647097998	11.7893547575055120	T	T	T
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6.7867605055091005	-0.5345848281743057	9.8530608420470678	T	T	T
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10.1498590505478283	-2.5464060249271436	9.8462738316990759	T	T	T
9.0439372133131748	-4.4780793610899439	8.2212220496627459	T	T	T
9.0631993249509986	-0.5514098990495313	8.1901896406605914	T	T	T
12.4043247463305590	-6.3706138823769098	8.2203297963196871	T	T	T
12.4254466905434757	-2.5361474071490138	8.1915463262467050	T	T	T
7.9437031651126695	-2.5177782483690980	6.6372662354529712	T	T	T
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6.8194402619999996	-0.5794706444999940	5.0875064650000468	F	F	F
10.1791603930000001	9.1192059670000063	5.0875064650000468	F	F	F
10.1791603930000001	-2.5192059664999937	5.0875064650000468	F	F	F
9.0592536826999606	-4.4589412888000286	3.5062484074000504	F	F	F
9.0592536826999606	-0.5794706443000290	3.5062484074000504	F	F	F
12.4189738136999601	-6.3986766108000284	3.5062484074000504	F	F	F
12.4189738136999601	-2.5192059663000288	3.5062484074000504	F	F	F
9.7881715445741317	8.2361136683192466	13.7023356694541114	T	T	T
13.1290652064609130	-3.4943695732637563	13.7017441288875901	T	T	T
12.6573216699370281	-7.2236006799627974	13.6463403293166063	T	T	T
9.2829694854080831	-3.6227203522398792	13.6641138707599108	T	T	T
11.2481676333443303	-4.9654307605400883	14.8365577948912950	T	T	T
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7.8685736929820456	9.6708873391679528	14.8286132971176414	T	T	T
7.8718341370245204	-1.1212102541623912	14.3118295875417889	T	T	T
4.4982775569120692	7.3313695631959037	13.5043307060747946	T	T	T
1.1260768661904588	0.7475995333659869	13.7316444713517694	T	T	T
1.1450270111605434	5.1255460408290592	13.5008743615243549	T	T	T
4.4720745831160889	3.9552923117517431	13.7398234936164183	T	T	T
4.4985982020092123	-0.4276155793803533	13.5038326835704119	T	T	T
1.1260879993388608	8.5056041361232673	13.7322185204459899	T	T	T
1.1447058659321043	12.8850688256536756	13.5006338983968934	T	T	T
4.4717236630674098	11.7145263292793249	13.7397749376968044	T	T	T
11.2189046507343111	7.3312380313595025	13.5038033386966738	T	T	T
7.8464028241769563	0.7470382948584451	13.7325970473797678	T	T	T
7.8648627591587106	5.1269249497433975	13.5026005686867201	T	T	T
11.1915641133109176	3.9564691354576098	13.7407162620471599	T	T	T
11.2187146388373034	-0.4288147903238988	13.5045225898217680	T	T	T
7.8460068597805401	8.5066189581855980	13.7324624380923517	T	T	T
7.8647009304817947	-2.6330294618726029	13.5001760923617411	T	T	T
11.1913104393908185	-3.8036549346406829	13.7390093140160712	T	T	T

VO2-ML-b/CeO2 (111)

1.0

13.4388805240000000	-7.7589412879999999	0.0000000000000000
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0.0000000000000000	0.0000000000000000	22.0000000000000000

Ce O V

48 128 16

Selective Dynamics
Cartesian

2.3160489601812078	3.2949443420255151	10.6154320966712223	T T T
2.3454879765748440	-0.5764669514436959	10.5458474052011972	T T T
5.6445712468441833	1.3770509095240815	10.5801671813994389	T T T
5.7177969228998062	-2.5387681444338774	10.6663733548733681	T T T
0.0878673753382388	3.2989195550863961	7.4377318091937497	T T T
0.0891673924792053	7.1819453441982315	7.4251341954944747	T T T
3.4483288018018756	1.3652779251239264	7.4187369848906890	T T T
3.4616274184918985	5.2339337416095288	7.4361780696286068	T T T
1.2199067103000385	5.2397353222999641	4.2969520308999307	F F F
1.2199067103000385	1.3602646777999645	4.2969520308999307	F F F
4.5796268413000378	3.3000000002999643	4.2969520308999307	F F F
4.5796268413000378	-0.5794706442000352	4.2969520308999307	F F F
2.3173026238430099	11.0507410638686316	10.6265659196447810	T T T
2.3475597949510991	7.1830366359412396	10.5448584335455813	T T T
5.6420384142322018	9.1404352569360015	10.5864994818118276	T T T
5.7204693650906382	5.2176938617228759	10.6686818022492513	T T T
0.0904109497676932	11.0567909684224635	7.4355022436005234	T T T
0.0900478231844135	14.9428685852595056	7.4250323969110195	T T T
3.4490952746319876	9.1254682528631399	7.4201330303522770	T T T
3.4603573287868632	12.9912963774832928	7.4384432421423803	T T T
1.2199067103000385	12.9986766112999650	4.2969520308999307	F F F
1.2199067103000385	9.1192059667999636	4.2969520308999307	F F F
4.5796268413000378	11.0589412892999661	4.2969520308999307	F F F
4.5796268413000378	7.1794706447999648	4.2969520308999307	F F F
9.0366804074396097	-0.5870099793136410	10.6275044584845730	T T T
9.0670563661151800	-4.4563069650357452	10.5429128128016121	T T T
12.3597047348877940	-2.4946086277380664	10.5876391177317579	T T T
12.4389150620385429	-6.4173931439250671	10.6688456286025239	T T T
6.8098706130191422	-0.5821281141852044	7.4353489602429930	T T T
6.8092942936185583	3.3035273235925211	7.4240756817653395	T T T
10.1681623295709951	-2.5123351848654596	7.4200593077757766	T T T
10.1801628904196253	1.3534798146531211	7.4387736859464422	T T T
7.9393469723000392	1.3602646782999637	4.2969520308999307	F F F
7.9393469723000392	-2.5192059662000359	4.2969520308999307	F F F
11.2990671033000396	-0.5794706437000361	4.2969520308999307	F F F
11.2990671033000396	-4.4589412882000357	4.2969520308999307	F F F
9.0379399302224943	7.1705566042080768	10.6276471027011272	T T T
9.0661459571738003	3.3040166006690459	10.5461953573801548	T T T
12.3631217169610093	5.2569638035602972	10.5794352373032456	T T T
12.4368575806762554	1.3408900665560335	10.6667350133842618	T T T
6.8099010951575387	7.1783063721848874	7.4389262339128877	T T T
6.8085637721701611	11.0610442839061811	7.4248556618430124	T T T
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10.1805186952509441	9.1120180406287936	7.4369234196123850	T T T
7.9393469723000392	9.1192059672999655	4.2969520308999307	F F F
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4.5551671471781248	-0.6240179305710449	11.8998757711678351	T T T
0.0509763089774457	3.3040910052154504	9.9458096741593423	T T T
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2.3119965490156247	3.3117251912829100	8.2106700324338622	T T T
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5.6960350879884194	1.3677347055452183	8.2099839911313932	T T T
5.7039001876392996	-2.52094971139670294	8.2008921333459206	T T T
1.2141098627137548	5.2385133542282674	6.6253320134400600	T T T
1.2210946438558892	1.3611252425419735	6.6271250718413288	T T T
4.5689933877135429	3.2976618650309337	6.6314068926419614	T T T
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0.0999999999999990	7.1794706445000411	5.0875064650000468	F F F
3.4597201309999992	1.3602646780000403	5.0875064650000468	F F F
3.4597201309999992	5.2397353225000405	5.0875064650000468	F F F
2.3398134206999597	3.3000000002000061	3.5062484074000504	F F F
2.3398134206999597	-0.5794706442999938	3.5062484074000504	F F F
5.6995335516999601	1.3602646782000059	3.5062484074000504	F F F
5.6995335516999601	-2.5192059662999942	3.5062484074000504	F F F
3.1911430515678023	0.5410154129290468	13.9018818508043154	T T T
6.1276658885590809	-3.2698723752078038	13.1455091908857113	T T T
6.1763351103607160	0.4781921251354087	13.8949694396447185	T T T
2.4493426353237941	4.1979351677909289	13.8494691161170618	T T T
4.7056338418463159	2.9006520212541620	14.7991402009882247	T T T
4.3798075886440087	-1.8936555564952677	14.3630785523950948	T T T
1.0407177170977517	1.9442657979061488	14.7571085620511102	T T T
1.1581938128953582	6.6927163643359284	14.2560291892939173	T T T
1.1031236357888412	13.0993431457642053	11.8580097400626538	T T T
1.5095865518620712	9.1336587872935588	11.9821836505955428	T T T
4.2819229668064587	10.9827638403296692	12.0499065844635442	T T T
4.5561849375424934	7.1359898028075044	11.8996712959786386	T T T
0.0477675160445215	11.0588165271868633	9.9431420045506300	T T T
0.0769053996276993	14.9451206958382912	9.9084117605789164	T T T
3.4417849347619049	9.1271085384292903	9.8201830433235546	T T T

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2.3111220068684757 11.0721318009228575 8.2046326136084300 T T T
2.3246576214717969 7.1646529785104933 8.1933549180815213 T T T
5.7013657247054921 9.1223719453295686 8.2060414300385851 T T T
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0.0999999999999999 14.9384119335000403 5.0875064650000468 F F F
3.4597201309999992 9.1192059670000400 5.0875064650000468 F F F
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6.1252372083999163 4.4953246753371072 13.1412359565587522 T T T
6.1798033691977610 8.2354432347214193 13.9035271095400077 T T T
2.4501441066496925 11.9600744914199879 13.8512151445656571 T T T
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4.3788969603007333 5.8653739136496590 14.3627036658790423 T T T
1.0423022724409927 9.7014964112460707 14.7568880208692974 T T T
1.1569027285567133 14.4557421178853183 14.2533973097228817 T T T
7.8217237383460825 1.4628420612732906 11.8608093867401774 T T T
8.2275641765922458 -2.5046208749025460 11.9828802754730148 T T T
11.0020373356585779 -0.6560344291287068 12.0497209314562070 T T T
11.2731664502467392 -4.5013123514927011 11.9011731706315640 T T T
6.7674753237664635 -0.5787832786712332 9.9428667498309515 T T T
6.8003845582033113 3.3048107256549129 9.9079640885857181 T T T
10.1595952962403544 -2.5111141016238836 9.8201517725580594 T T T
10.2068153719897428 1.3534594717667607 9.9069949352914009 T T T
9.0298698103028929 -0.5658393784302058 8.2043051464226249 T T T
9.0426980125843048 -4.4733995533556730 8.1926805954603470 T T T
12.4196493972351867 -2.5143775281196525 8.2057962569728531 T T T
12.4280441189906874 -6.3982626808481875 8.1997298161977454 T T T
7.9286814434946278 1.3602011261887119 6.6252480425550839 T T T
7.9375930937738213 -2.5190204393188207 6.6271121343180406 T T T
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6.8194402619999996 3.3000000005000407 5.0875064650000468 F F F
10.1791603930000001 -2.5192059659999595 5.0875064650000468 F F F
10.1791603930000001 1.3602646785000410 5.0875064650000468 F F F
9.0592536826999606 -0.5794706437999944 3.5062484074000504 F F F
9.0592536826999606 -4.4589412882999948 3.5062484074000504 F F F
12.4189738136999601 -2.5192059657999941 3.5062484074000504 F F F
12.4189738136999601 -6.3986766102999946 3.5062484074000504 F F F
9.9129299592925015 -3.3394812380803081 13.9060292132145431 T T T
12.8454482365951375 -7.1454106098664871 13.1449846400848518 T T T
12.8977806018090018 -3.4022136814406929 13.9026459529882480 T T T
9.1693860799387608 0.3194579377274982 13.8500701265071591 T T T
11.4296851680957605 -0.9712694835123887 14.8110390019592426 T T T
11.0961645025934263 -5.7717638860454796 14.3638902627071801 T T T
7.7605508727498851 -1.9366732523035632 14.7578092707324391 T T T
7.8769371214837829 2.8168077304257944 14.2560210816611779 T T T
7.8221535563003517 9.2227264244019231 11.8605754879407215 T T T
8.2326960425958831 5.2543604338186567 11.9863840792986167 T T T
10.9986962431892739 7.0977139037872581 12.0561443969364195 T T T
11.2718426966865444 3.2537461659659037 11.9013586646234248 T T T
6.7714483617891092 7.1767078375076370 9.9422093803070375 T T T
6.7953774217175988 11.0661725419192507 9.9066047185456636 T T T
10.1607542732624108 5.2440307495689380 9.8218011355919703 T T T
10.2104906260351775 9.1115050310233343 9.9084755897297239 T T T
9.0337542576054695 7.1927111118081744 8.2045164574978724 T T T
9.0447430791931112 3.2857206420530121 8.1904509388619395 T T T
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12.4234064383563503 1.3580414674041741 8.2011080546663475 T T T
7.9324943961697532 9.1189507177210878 6.6246219999264513 T T T
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11.2913454126976820 7.1787232952272744 6.6317455373306107 T T T
11.2955399543538739 3.3038695217930973 6.6345916104212339 T T T
6.8194402619999996 7.1794706450000403 5.0875064650000468 F F F
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10.1791603930000001 5.2397353230000405 5.0875064650000468 F F F
10.1791603930000001 9.1192059675000401 5.0875064650000468 F F F
9.0592536826999606 7.1794706452000057 3.5062484074000504 F F F
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12.4189738136999601 1.3602646787000063 3.5062484074000504 F F F
9.9157613931869300 4.4178085683733368 13.9077827359020212 T T T
12.8482325561273054 0.6092770875068929 13.1438001725732772 T T T
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9.1691606592197186 8.0811717500792906 13.8531455884060826 T T T
11.4326127952495931 6.7847912357154110 14.8116055593046116 T T T
11.0989992336981516 1.9823073625387622 14.3648293081836087 T T T
7.7582244242516349 5.8228908261490222 14.7607760212891481 T T T
7.8774531372494350 10.5732719444824959 14.2575826717677714 T T T

4.5746651114375636	-0.3706811768642200	13.6298379525979332	T	T	T
1.1549171845777189	0.7996300441454188	13.6386400399408139	T	T	T
1.0411515679017291	5.1296777959708919	13.5826587499076155	T	T	T
4.4064412936325077	3.9876097150686496	13.6650286136740924	T	T	T
4.5772192023432350	7.3862226864323883	13.6305086821776520	T	T	T
1.1541357785690181	8.5557550970428888	13.6392520820600005	T	T	T
1.0427394534148240	12.8905381206329999	13.5819260122631196	T	T	T
4.4153049704654643	11.7492342047718914	13.6712412395246847	T	T	T
11.2948046244521745	-4.2507337525289159	13.6312897481497313	T	T	T
7.8733975026398886	-3.0823296157792273	13.6403259573783178	T	T	T
7.7624231064388711	1.2520300957245070	13.5840162687703945	T	T	T
11.1344293231596758	0.1115205182938332	13.6717503237499063	T	T	T
11.2947023838021323	3.5064729375663237	13.6313918803063352	T	T	T
7.8649493450973944	4.6781146594225413	13.6411943322917484	T	T	T
7.7619465525242557	9.0096690968345285	13.5843810744591096	T	T	T
11.1358110183448673	7.8670166791720240	13.6721332471308106	T	T	T

VO2-ML-c/CeO2 (111)

1.0		
13.4388805240000000	-7.7589412879999999	0.0000000000000000
0.0000000000000000	15.5178825780000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.0000000000000000

Ce O V

48 128 16

Selective Dynamics

Cartesian

2.2992954972223907	3.2983480761826613	10.6036185042026077	T	T	T
2.3004954170110472	-0.5804976625760250	10.6025091476564963	T	T	T
5.7024252810565486	1.3587929847170814	10.6104695288917092	T	T	T
5.7043107362586891	-2.5198875880392402	10.5967811691678673	T	T	T
0.0969613174904094	3.3013574561952708	7.4263999539235810	T	T	T
0.0946323687475236	7.1796660641956986	7.4279814371107928	T	T	T
3.4611039163201474	1.3595201442433713	7.4317340372199014	T	T	T
3.4591624557166334	5.2387690165086553	7.4291399018973889	T	T	T
1.2199067103060550	5.2397353223021144	4.2969520309099360	F	F	F
1.2199067103060550	1.3602646778021148	4.2969520309099360	F	F	F
4.5796268413060544	3.3000000003021146	4.2969520309099360	F	F	F
4.5796268413060544	-0.5794706441978850	4.2969520309099360	F	F	F
2.3017634633694715	11.0583505942438585	10.6031479095141901	T	T	T
2.3006689247638477	7.1783991056099143	10.6021482775239662	T	T	T
5.7035373063846047	9.1181008174591263	10.5973757784056293	T	T	T
5.7019159565137567	5.2368225625468909	10.5944433924308594	T	T	T
0.0955885062221525	11.0579474056053346	7.4278252065167782	T	T	T
0.0968740691407100	14.9355210962121969	7.4261456406945152	T	T	T
3.4595811917207793	9.1189564482085981	7.4291966886244607	T	T	T
3.4602277452749410	12.9982267467764476	7.4292695947333840	T	T	T
1.2199067103060550	12.9986766113021144	4.2969520309099360	F	F	F
1.2199067103060550	9.1192059668021148	4.2969520309099360	F	F	F
4.5796268413060544	11.0589412893021155	4.2969520309099360	F	F	F
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9.0189609247823022	-0.5792152933213499	10.6004231451249282	T	T	T
9.0199802661320145	-4.4597306640734891	10.6045388713148885	T	T	T
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12.4246835609329711	-6.3998336471231250	10.5933468433846532	T	T	T
6.8157516556490663	-0.5775806390161895	7.4272086976451739	T	T	T
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10.1805680851932401	-2.5192946387369406	7.4312051447361371	T	T	T
10.1798248463528846	1.3602605032965469	7.4308112779697746	T	T	T
7.9393469723060548	1.3602646783021148	4.2969520309099360	F	F	F
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11.2990671033060543	-0.5794706436978858	4.2969520309099360	F	F	F
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9.0206588661627372	7.1761183676064766	10.6025179619808227	T	T	T
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4.8374459883093488	-0.5841528333183739	11.9640054627282293	T	T	T
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2.3398134207021557	3.3000000001974139	3.5062484073980174	F	F	F
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5.6995335517021557	-2.5192059663025854	3.5062484073980174	F	F	F
3.7371119678104678	1.3578957858069676	13.7046399322740307	T	T	T
2.2507869534141265	-0.5809827757575011	13.3972952252612689	T	T	T
2.2517817378131064	3.2976966867386874	13.3960558415748654	T	T	T
3.7398876842535995	5.2347239164026913	13.7018094376346333	T	T	T
5.3752999898278988	-0.5792911142442252	14.7200445824446362	T	T	T
0.7538183677296246	1.3588012552938733	14.7091542511980329	T	T	T
5.3725631908668987	3.2959337364933949	14.7235026189868492	T	T	T
0.7557266702576714	5.2339529942643592	14.7113616372955960	T	T	T
1.1114858038718469	12.9957248760876904	11.8807448761876078	T	T	T
1.1129639734924601	9.1169047959820908	11.8813626333707134	T	T	T
4.8427867757612573	11.0590427683028611	11.9665160025430470	T	T	T
4.8305260706999791	7.1785951719514669	11.9572404408402342	T	T	T
0.1180604147090832	11.0571444894925488	9.8336789218995317	T	T	T
0.1144185849000851	14.9375462489995954	9.8368169833776591	T	T	T
3.4417594161250720	9.1188445144962316	9.9559280143019890	T	T	T
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2.3654632443333075	11.0586935565203248	8.2033151983280916	T	T	T
2.3643785413532550	7.1797094626992397	8.2031574985669948	T	T	T
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1.2184156746473140	12.9981949734486193	6.6374275488053591	T	T	T
1.2186648688950890	9.1190489353848641	6.6375368087140094	T	T	T
4.5849173865120791	11.0588370558337665	6.6248359149952583	T	T	T
4.5838226607924986	7.1802638481461019	6.6239425911721792	T	T	T
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2.2518081459817796	7.1771795381365227	13.4039638525050417	T	T	T
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3.7391630235299282	13.0007729583494918	13.7041409215909873	T	T	T
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7.8229121842094616	1.3592106043329979	11.8924772352417918	T	T	T
7.8245830672370236	-2.5186325580574289	11.8818629006981897	T	T	T
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10.1609343606534956	1.3607704812833168	9.9506375096112478	T	T	T
9.0802616599076238	-0.5804377874504780	8.2042313264618301	T	T	T
9.0813954592119934	-4.4620922763993054	8.2056325127950274	T	T	T
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12.3967159806401099	-6.3985783360713064	8.2059929444659296	T	T	T
7.9344651676778843	1.3567698975531828	6.6366555695935450	T	T	T
7.9357187067457078	-2.5210413795828610	6.6384587886378679	T	T	T
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11.3010016609562634	-4.4612130349336185	6.6237670648058815	T	T	T
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10.1791603930041052	-2.5192059660079522	5.0875064650080200	F	F	F
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9.0592536827021561	-0.5794706438025861	3.5062484073980174	F	F	F
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12.4189738137021557	-2.5192059658025858	3.5062484073980174	F	F	F
12.4189738137021557	-6.3986766103025854	3.5062484073980174	F	F	F
10.4561501695035570	-2.5201601332585732	13.7083007450591996	T	T	T
8.9713117605860599	-4.4611547833096621	13.3958025953720448	T	T	T
8.9706850651835754	-0.5807982818684181	13.4017055079325385	T	T	T
10.4564404370218469	1.3536147561912415	13.7154644216818831	T	T	T
12.0914851787924480	-4.4632110436328283	14.7252994590017519	T	T	T
7.4700399224905167	-2.5243580946803990	14.7077013078850793	T	T	T
12.0862165731439060	-0.5867179226166392	14.7344865922830213	T	T	T
7.4788372707009811	1.3588957450578087	14.7201017850367393	T	T	T
7.8234615360347277	9.1151596862050539	11.8828173466883591	T	T	T
7.8191055077461025	5.2338137200799917	11.8914776971282627	T	T	T
11.5609930448729656	7.1819780196107503	11.9702711825991415	T	T	T
11.5830266078301385	3.2955101056097611	11.9921099006374536	T	T	T
6.834723932824486	7.1767115865386781	9.8418515455731104	T	T	T
6.8343860348912040	11.0588794746349155	9.8410925467970003	T	T	T
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9.0815465842217016	7.1817107149987018	8.2047121884609062	T	T	T
9.0737505385677206	3.2982277221982121	8.1955375189509727	T	T	T
12.3969525854813423	5.2390862070609607	8.1986805635389892	T	T	T
12.3966367706922238	1.3594323708735363	8.1978763207404590	T	T	T
7.9351866733531411	9.1191902483611536	6.6373017151830833	T	T	T
7.9347478659691335	5.2426551005742921	6.6374588894127466	T	T	T
11.3017241169351514	7.1812535328974425	6.6242212437785843	T	T	T
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6.8194402620041057	7.1794706449920476	5.0875064650080200	F	F	F
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10.1791603930041052	5.2397353229920478	5.0875064650080200	F	F	F
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9.0592536827021561	7.1794706451974148	3.5062484073980174	F	F	F
9.0592536827021561	3.3000000006974153	3.5062484073980174	F	F	F
12.4189738137021557	5.2397353231974151	3.5062484073980174	F	F	F
12.4189738137021557	1.3602646786974155	3.5062484073980174	F	F	F
10.4584678175617167	5.2363450312357367	13.7081770459789425	T	T	T
8.9781883456975464	3.2948938714276954	13.3988129886845186	T	T	T
8.9715649627957710	7.1749112657700902	13.4025988543594536	T	T	T
10.4569215099296962	9.1171727510675389	13.7071859909294691	T	T	T
12.0712929073472441	3.2948977355847742	14.7586309850155573	T	T	T
7.4813206875572051	5.2320416010827469	14.7198010585947330	T	T	T
12.0904554639515691	7.1774132247874673	14.7286640849416841	T	T	T
7.4703249692928591	9.1193716181487261	14.7085541884421929	T	T	T
4.2269405916976917	3.2983085927146636	13.6035122830891027	T	T	T
1.8112725702205927	5.2381608555118984	13.5110940029048585	T	T	T
1.8084802509269482	1.3596103149217846	13.5083110041437973	T	T	T
4.2269051409571743	-0.5828587568095851	13.6029361422603365	T	T	T
4.2278584066429881	11.0565171360147154	13.6051789908917673	T	T	T
1.8108598648306962	12.9994408871834004	13.5097851717667705	T	T	T
1.8116112825786517	9.1179832972190056	13.5103747304125807	T	T	T
4.2280404336034145	7.1792888744347145	13.6004579933841363	T	T	T
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8.5268514579781538	-2.5244341859154917	13.5091259853479269	T	T	T
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10.9469466585523811	7.1852780232982880	13.6070667624340267	T	T	T
8.5266231498033669	9.1181182758581105	13.5096060542860670	T	T	T
8.5298691101582769	5.2412040754582216	13.5142119551292499	T	T	T
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V16031/CeO2 (111)

1.0

13.4388805240000000	-7.7589412879999999	0.0000000000000000
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Selective Dynamics

Cartesian

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5.6974012420315177	5.2215407315505287	10.5246198571029677	T	T	T
0.1124240200471259	3.2922856583907754	7.4412693971812907	T	T	T
0.0836065411189883	7.1980841212855013	7.4281212573223083	T	T	T
3.4644582741517578	1.3844696064764364	7.4297171602931602	T	T	T
3.4427650932985059	5.2296480681363340	7.4272502157977041	T	T	T
1.2199067099969567	5.2397353218288183	4.2969520308000417	F	F	F
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4.5796268409969567	3.2999999998288181	4.2969520308000417	F	F	F
4.5796268409969567	7.1794706443288181	4.2969520308000417	F	F	F
2.3552151339255025	11.0606687022999068	10.6948645050464339	T	T	T
2.3584750626658422	-0.5378746262032722	10.5411379386488431	T	T	T
5.7166052588357923	9.1274435788959121	10.6841944219158407	T	T	T
5.6891987879267809	-2.5449853608933042	10.5234867511260060	T	T	T
0.1125631959883415	11.0468872515567540	7.4363152272783664	T	T	T
0.0946027353466313	14.9580870163717208	7.4323102563361978	T	T	T
3.4683554749607568	9.1397830477723438	7.4347178488117880	T	T	T
3.4444333719864475	12.9875010247195579	7.4267886353675365	T	T	T
1.2199067099969567	12.9986766108288183	4.2969520308000417	F	F	F
1.2199067099969567	9.1192059663288187	4.2969520308000417	F	F	F
4.5796268409969567	11.0589412888288177	4.2969520308000417	F	F	F
4.5796268409969567	-0.5794706446711815	4.2969520308000417	F	F	F
9.0881448750385090	3.2932835111004470	10.6514297289169484	T	T	T
9.0585896846431435	7.1936669095333849	10.5289275516681133	T	T	T
12.4194570327542468	1.3771245002212220	10.6880624206763493	T	T	T
12.4276111307322878	5.2267982110067601	10.5354158113113545	T	T	T
6.8319739616844064	3.2898915588344049	7.4248356692020590	T	T	T
6.8046873638420697	7.1945827872174082	7.4257362826956328	T	T	T
10.1930665492671739	1.3787465706423214	7.4268989598598214	T	T	T
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7.9393469719969572	5.2397353223288183	4.2969520308000417	F	F	F
7.9393469719969572	1.3602646778288179	4.2969520308000417	F	F	F
11.2990671029969576	3.3000000003288186	4.2969520308000417	F	F	F
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9.0881321409336842	-4.4844680352180184	10.6593422257473200	T	T	T

9.0346066021836311	-0.5772323268295398	10.4808559720418888	T	T	T
12.4525258548893518	-6.3845160434569781	10.6914723016840654	T	T	T
12.4036056315012289	-2.5181570802334203	10.5504628575624579	T	T	T
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7.9393469719969572	9.1192059668288188	4.2969520308000417	F	F	F
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11.2990671029969576	-0.5794706441711819	4.2969520308000417	F	F	F
1.1480844735384408	5.4685177545541404	11.7931181543363159	T	T	T
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5.7026982037840979	5.2229288127178215	8.1846184468958896	T	T	T
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6.0050801089870225	0.6109873870232363	13.8969896468294412	T	T	T
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1.1824604136892525	13.2172589846617967	11.7831457065281811	T	T	T
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4.6477222069426167	-0.6641343880691952	11.8324023095004591	T	T	T
0.1178889815657003	11.0230277986422465	9.9519233813479744	T	T	T
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1.2267329142221870	13.0017953526689460	6.6344328172583529	T	T	T
1.2147892574844514	9.1256315026329418	6.6262625392258379	T	T	T
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5.6995335522261996	-2.5192059668379030	3.5062484071999624	F	F	F
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9.0592536832261992	7.1794706446620964	3.5062484071999624	F	F	F
12.4189738142262005	1.3602646781620971	3.5062484071999624	F	F	F
12.4189738142262005	5.2397353226620966	3.5062484071999624	F	F	F
9.7682012358808041	0.6182842603541419	13.9512653236810102	T	T	T
13.1421723863759876	4.2590135919533871	13.6651979555824958	T	T	T
12.6511372850087920	0.4622484175307440	13.7284941565771064	T	T	T
9.2662201159132476	4.0541764427920013	13.7294680639493922	T	T	T
11.3163761413185657	2.8182768740577462	14.8786636333208726	T	T	T
11.1833130073530604	5.8055832261822520	14.3007297441962145	T	T	T
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6.7769643821377104	-0.5590361927618113	9.8073614767078858	T	T	T
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9.0539949746270203	-4.4881768520599561	8.2139377497765373	T	T	T
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12.4301177320238718	-2.5342696683643782	8.1959584968943204	T	T	T
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9.0592536832261992	-4.4589412888379032	3.5062484071999624	F	F	F
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1.1522081289333770	5.1319388209735095	13.5060488230069691	T	T	T
4.4749419483501160	3.9461782548064384	13.7364046125867851	T	T	T
4.5867160560406379	-0.3839495409933824	13.5591286630281687	T	T	T
1.1146289120381470	8.4823773184333042	13.7499131989812096	T	T	T
1.1562258714751597	12.8919043033987784	13.4993096431900099	T	T	T
4.4871242696088158	11.7033444374427784	13.7301047389565269	T	T	T
11.2384905829047579	7.3254847448555198	13.4903057552296328	T	T	T
7.8895796226726054	0.6323906370466261	13.6204335033431700	T	T	T
7.8780011581810836	5.0759475538084917	13.5104161421507420	T	T	T
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7.8562344778881421	8.4748098971938859	13.7280992743007637	T	T	T
7.8821574370883516	-2.7429383242258094	13.4076595018335283	T	T	T
11.2066176950041410	-3.8226605315327542	13.7253893944844556	T	T	T

V205-ML-a/CeO2 (111)

1.0

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Ce O V

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Selective Dynamics

Cartesian

2.3707025945689200	3.2913681089555364	10.6794779563039306	T	T	T
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5.7367506541676043	-2.5902970513800385	10.4972569515583150	T	T	T
0.0981647099442542	3.3042821743046038	7.4433034340531927	T	T	T
0.1098192881477305	7.1707765837593849	7.3947743900377221	T	T	T
3.4637697313710749	1.3523237373405446	7.4455112306787559	T	T	T
3.4594425389166013	5.2420298708784054	7.4393995823610073	T	T	T
1.2199067059653168	5.2397352636367671	4.2969519999999628	F	F	F
1.2199067059653168	1.3602646191367684	4.2969519999999628	F	F	F
4.5796268504042459	3.2999999338777983	4.2969519999999628	F	F	F
4.5796268504042459	-0.5794707106222008	4.2969519999999628	F	F	F
2.3704481761715264	11.0500823885604138	10.6799403808565199	T	T	T

2.2946147519033064	7.1712441899912509	10.5874751886911262	T T T
5.7230800610558132	9.1787391310530957	10.5791986840641279	T T T
5.7364908988630461	5.1685403003867396	10.4966822825698891	T T T
0.0981763928273559	11.0630765431467317	7.4434734155028321	T T T
0.1100245275326081	14.9297281053041804	7.3944402881285711	T T T
3.4635296412127619	9.1113358636261719	7.4456573095232113	T T T
3.4595912794566699	13.0010125275327866	7.4394493537196560	T T T
1.2199067059653168	12.9986765526367680	4.2969519999999628	F F F
1.2199067059653168	9.1192059081367685	4.2969519999999628	F F F
4.5796268504042459	11.0589412228777988	4.2969519999999628	F F F
4.5796268504042459	7.1794705783777992	4.2969519999999628	F F F
9.0898658136056145	-0.5883719062342898	10.6796301660889927	T T T
9.0143703423923167	-4.4673243069405277	10.5870169064137780	T T T
12.4425267805074693	-2.4597515571066193	10.5798916080034875	T T T
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6.8176389579912566	-0.5752705157808005	7.4433399734394268	T T T
6.8293717052978309	3.2911773306750800	7.3945547280234276	T T T
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7.9393469814042454	1.3602646118777981	4.2969519999999628	F F F
7.9393469814042454	-2.5192060326222010	4.2969519999999628	F F F
11.2990671124042450	-0.5794707101222016	4.2969519999999628	F F F
11.2990671124042450	-4.4589413546222012	4.2969519999999628	F F F
9.0902571604081857	7.1705363482384827	10.6797937364789473	T T T
9.0144013145226438	3.2917574848502804	10.5871576894279507	T T T
12.4429614167233069	5.2993524446040601	10.5789935816297564	T T T
12.4559012003691301	1.2891176727774170	10.4976340348346913	T T T
6.8175151576053663	7.1837221281881627	7.4434010916871847	T T T
6.8292706769823788	11.0503824145687943	7.3945493115430736	T T T
10.1830479053046563	5.2318549637084448	7.4456248782803494	T T T
10.1789189330347583	9.1215355452118967	7.4394327819941646	T T T
7.9393469814042454	9.1192059008777981	4.2969519999999628	F F F
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1.2769444836204642	5.2315606861334336	11.1971468335464799	T T T
1.2276716179900642	1.3872872072482698	11.1634156099370365	T T T
4.5657980966540945	3.3253937266451308	11.1472200669660229	T T T
4.4940049182859072	-0.7445854324869201	11.8048089081326637	T T T
6.6278047640693778	-0.5597101969077620	9.8227044438866162	T T T
6.8371759594944042	3.2725532489717493	9.7627599245716628	T T T
3.5665128111944941	1.1916926570568034	9.8411944298907006	T T T
3.5386826358595980	5.3742768662308311	9.7709052490209558	T T T
2.3336949562442553	3.2777964591864124	8.3604813020002755	T T T
2.3112044588355412	-0.5699186637981404	8.1933745655949739	T T T
5.71337701282117506	1.3916883465605223	8.1872883517236428	T T T
5.7343787140137943	-2.5535805919687271	8.1835588363401595	T T T
1.2410863198548088	5.2068752978353148	6.6363317705658842	T T T
1.2393001439415354	1.3897394388038606	6.6278204479402190	T T T
4.5442277513192195	3.3013744084360481	6.6343804306774059	T T T
4.5831251724159499	-0.5837137249311466	6.6516857599262265	T T T
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0.1000000001116264	7.1794706866695970	5.0875063799999642	F F F
3.4597201848671526	1.3602646891338295	5.0875063799999642	F F F
3.4597201848671526	5.2397353336338295	5.0875063799999642	F F F
2.3398133849412437	3.3000000113005510	3.5062484599999668	F F F
2.3398133849412437	-0.5794706176816206	3.5062484599999668	F F F
5.6995335159412432	1.3602646893005512	3.5062484599999668	F F F
5.6995335159412432	-2.5192059396816204	3.5062484599999668	F F F
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V16039/CeO2 (111)

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V16038/CeO2 (111)

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Ce O V
48 134 16

Selective Dynamics
Cartesian

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