SUPPORTING INFORMATION

A Universal Approach to Quantify Overpotential-Dependent Selectivity Trends for the Competing Oxygen Evolution and Peroxide Formation Reactions: A Case Study on Graphene Model Electrodes

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Section 1. Relaxed geometries of systems with adsorbed RIs

We modeled different densities of active centers of adsorption by changing the supercell's size. **Figure S1** shows bare surfaces of graphene used in this study. Different sizes of supercells

represent different concentration of adsorbed RIs (G2 – 50%, G4 – 25%, G6 – 17%, G8 – 12.5%, G12 – 8.3%, G16 – 6%, G24 – 4%, G32 – 3%). This allowed us to model properties of a graphene electrode as a function of adsorbed RIs' concentration. We placed a single adsorbate species in a supercell at an initial distance of ~2 Å away from the surface and allowed a full relaxation of the system. HO* and HOO* adsorb on top of a carbon atom forming a covalent bond, while O* adsorbs in bridge position, interacting with 2 carbon atoms simultaneously. **Table S1** lists structural features of the relaxed systems.

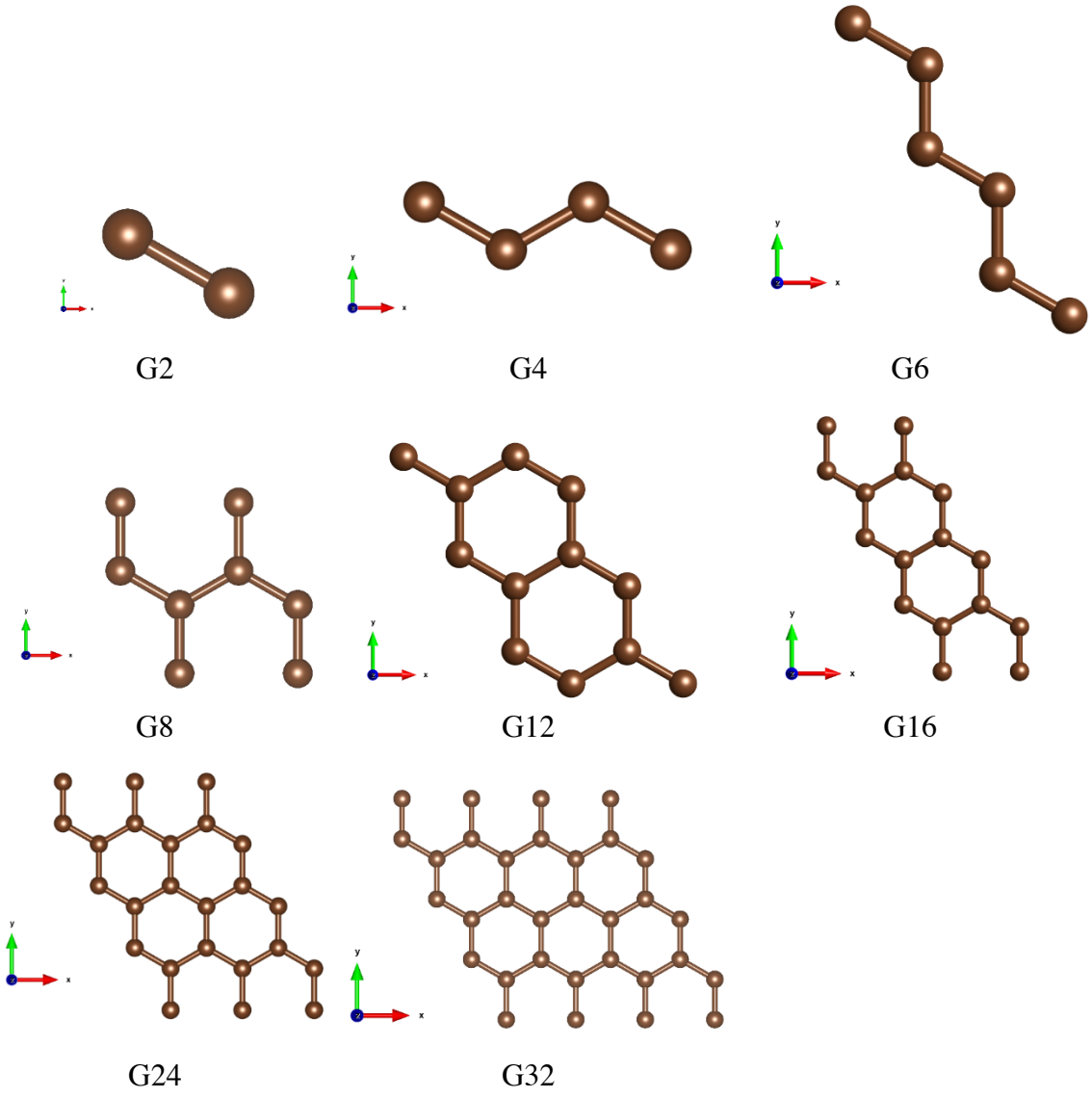
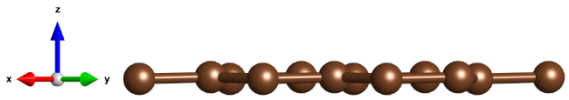
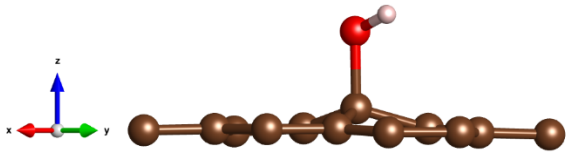
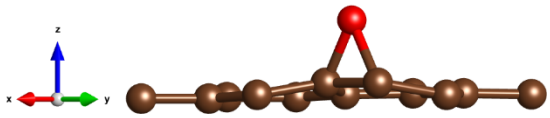
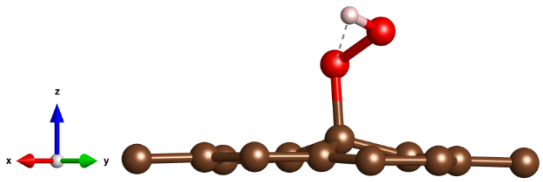


Figure S1. Optimized structures of pristine graphene surfaces.

Table S1. Relaxed geometries of systems with adsorbed RIs and their parameters.

Model	Optimized geometry	C–C bond length, Å	C–O bond length, Å	O–C–C angle ,°
G12		1.411	–	–
G12-HO*		~1.487	1.486	103.2 105.6 106.5
G12-O*		~1.469	1.461	~59.6 ~112.6
G12-HOO*		~1.480	1.523	97.9 106.0 107.6

Section 2. Computational optimization scheme

In the work of Gebhardt et al., the VASP program package was used, which uses non-hybrid DFT functionals in order to manage computational costs.[1] Even nowadays, hybrid calculations with VASP are resource demanding. On the other hand, the CRYSTAL code, which utilizes the LCAO approximation, allows the use of hybrid functionals. The computational scheme around

HSE06 was optimized for the diamond structure, as future applications of this scheme involve BDD simulations. In order to explain the choice of our computational scheme, we provide data on the screening of different functionals and basis sets (cf. **Table S2**). The value of the diamond bandgap evaluated with HSE06 has the smallest relative error regardless of the chosen basis set.

Table S2. Computational optimization scheme.

Basis set	**Functional**	**a, Å**	**Relative error, %**	**Band gap, eV**	**Relative error, %**	**CPU time, h**
C_m-6-311G(d)	B3LYP	3.573	0.17	5.94	8.53	3.27
_Heyd_2005	PBE0	3.549	0.52	6.04	10.35	3.39
	HSE06	3.549	0.50	5.36	2.03	4.66
	B3PW	3.555	0.33	5.73	4.72	2.80
	B1WC	3.544	0.64	5.33	2.48	2.10
	HSEsol	3.537	0.83	5.30	3.15	5.27
	PBE	3.574	0.20	4.14	24.25	0.18
	PBESOL	3.556	0.29	4.05	25.99	0.05
C_pob_	B3LYP	3.567	0.00	5.99	9.56	0.09
TZVP_2012	PBE0	3.543	0.67	6.08	11.18	0.84
	HSE06	**3.544**	**0.64**	**5.40**	**1.19**	**0.96**
	B3PW	3.550	0.48	5.77	5.45	0.47
	B1WC	3.539	0.78	5.37	1.91	0.62
	HSEsol	3.533	0.95	5.34	2.45	1.20
Experimental values		3.567	Ref.[2]	5.47	Ref.[3]	

Section 3. Binding energy analysis

In order to prove the suitability of our models as well as to estimate lateral interaction effects of absorbed intermediates, we conducted a binding energy (BE) analysis. BE of reaction intermediate (RI) was calculated by eq. (S1), using the total energies of the systems obtained from DFT calculations. The models were constructed to represent different active-site concentrations on the graphene surface (see **Section 1** of the SI). BEs are displayed in **Figure S2** as a function of the number of carbon atoms in a single unit cell. It can be seen that the G2 model with 50% coverage is an outlier, which is an expected result because the unit cell area is too small to host RIs. For this particular reason, the G2 model is excluded from the further analysis. **Figure S2** shows that BE_{HO*} is lower than BE_{O*}, but both are negative so both can adsorb to graphene with a release of energy. On the other hand, BE_{HOO*} is positive for all models, which means repulsion between the interacting components, or in other words, energy needs to be supplied to allow adsorption of HOO*.

$$BE_{RI} = E_{\frac{RI}{graphene}} - E_{radical} - E_{graphene} \quad \text{(S1)}$$

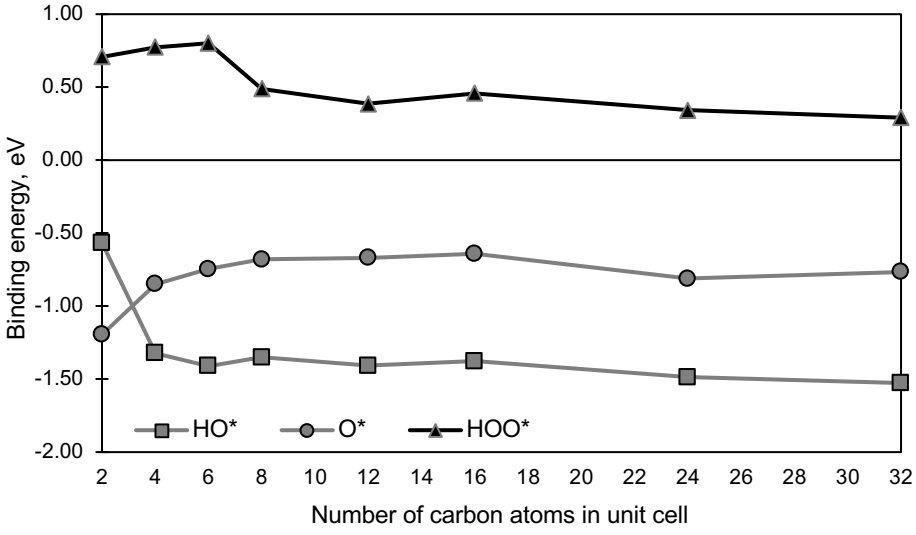


Figure S2. The binding energies of HO*, O* and HOO* intermediates on a graphene surface with different coverages.

By analyzing relaxed geometries of systems with adsorbed RIs, we can get chemical insights about the catalytic process. The graphene structure is a plane consisting of sp^2-hybrid carbon atoms, where each atom has three sigma bonds with pairwise bond angles of 120°. Adsorption of RIs causes structural changes in that graphene adjusts to interact with the intermediate. Carbon atoms that interact with the RI ceases to be planar and adopt tetrahedral geometry. This is evidenced by values of O-C-C dihedral angles in relaxed structures, which are close to standard tetrahedral carbon geometry (109.5°). This observation suggests that a covalent bond is formed between a carbon atom and an oxygen atom, accompanied by a change of carbon's hybridization from sp^2 to sp^3. In other words, oxygen-containing RIs adsorb to graphene via chemisorption. The change of hybridization in theoretical calculations was reported by Jiao et al., which proves the adequacy of the present model.[4]

Section 4. Free-energy diagram for the WOR at non-zero applied electrode potential

Mechanism of the water-oxidation reaction (WOR) used in this paper:

1e⁻ WOR (U_{eq} = 2.38 V *vs*. RHE):

$$H_2O(l) + * \leftrightarrow HO \cdot (aq) + * + H^+ + e^-$$

2e⁻ WOR (U_{eq}^{PER} = 1.76 V *vs*. RHE):

$$H_2O(l) + * \leftrightarrow HO* + H^+ + e^-$$

$$HO* + H^+ + e^- + H_2O(l) \leftrightarrow H_2O_2(l) + * + 2(H^+ + e^-)$$

4e⁻ WOR (U_{eq}^{OER} = 1.23 V *vs*. RHE):

$$H_2O(l) + * \leftrightarrow HO* + H^+ + e^-$$

$$HO* + H^+ + e^- \leftrightarrow O* + 2(H^+ + e^-)$$

$$O* + 2(H^+ + e^-) + H_2O(l) \leftrightarrow HOO* + 3(H^+ + e^-)$$

$$HOO* + 3(H^+ + e^-) \leftrightarrow O_2(g) + * + 4(H^+ + e^-)$$

According to the presented mechanism, free-energy profiles were calculated for high and low coverage modes. **Table S3** presents the values of ΔG_* that were calculated as average across all models with high (> 17%) or low coverage (≤12.5%) at different values of the applied electrode potential *vs*. SHE (standard hydrogen electrode) at pH = 0.

Table S3. ΔG_* values for the reaction intermediates of the 4 e⁻ WOR, calculated at different $@U$ values and pH = 0.

RI high coverage 17 % – 25 %							
@U=0V		**@U=1.23V**		**@U=1.23V**		**@U=1.76V**	
RI	ΔG_*, eV	RI	ΔG_*, eV	RI reordered	ΔG_*, eV	RI	ΔG_*, eV
H_2O+*	0.00	**H_2O+***	0.00	**O***	0.00	**O***	0.00
HO*	2.82	**HO***	1.59	**HOO***	1.00	**HOO***	0.47
O*	0.97	**O***	-1.49	**O_2+***	1.49	**O_2+***	0.43
HOO*	3.19	**HOO***	-0.50	**HO***	3.09	**HO***	1.50
O_2+*	4.92	**O_2+***	0.00	**O***	0.00	**O***	0.00
HO*	2.82	**HO***	1.59	**HO***	1.59	**HO***	1.00
HO (aq)	4.19	**HO (aq)**	2.96	**HO (aq)**	2.96	**HO(aq)**	2.43
H_2O_2	3.52	**H_2O_2**	1.06	**H_2O_2**	1.06	**H_2O_2**	0
RI low coverage 3 % – 12.5 %							
@U=0V		**@U=1.23V**		**@U=1.23V**		**@U=1.76V**	
RI	ΔG_*, eV	RI	ΔG_*, eV	RI reordered	ΔG_*, eV	RI reordered	ΔG_*, eV
H_2O+*	0.00	**H_2O+***	0.00	**O***	0.00	**HOO***	0.00
HO*	2.76	**HO***	1.53	**HOO***	0.37	**O_2+***	0.44
O*	1.11	**O***	-1.35	**O_2+***	1.35	**HO***	1.44
HOO*	2.72	**HOO***	-0.97	**HO***	2.88	**O***	-1.96
O_2+*	4.92	**O_2+***	0.00	**O***	0.00	**HOO***	-2.12
HO*	2.76	**HO***	1.53	**HO***	1.53	**HO***	1.06
HO (aq)	4.19	**HO (aq)**	2.96	**HO (aq)**	2.96	**HO (aq)**	2.43
H_2O_2 +*	3.52	**H_2O_2 +***	1.06	**H_2O_2 +***	1.06	**H_2O_2 +***	0

Figure S3 displays the free-energy diagrams for three competing one-, two- and four-electron processes at zero electrode potential ($@U$ = 0 V *vs*. SHE). Different adsorbate coverage

concentrations do not influence the general trends in the free-energy landscape; thus, the free-energy profile is depicted for low adsorbate coverage.

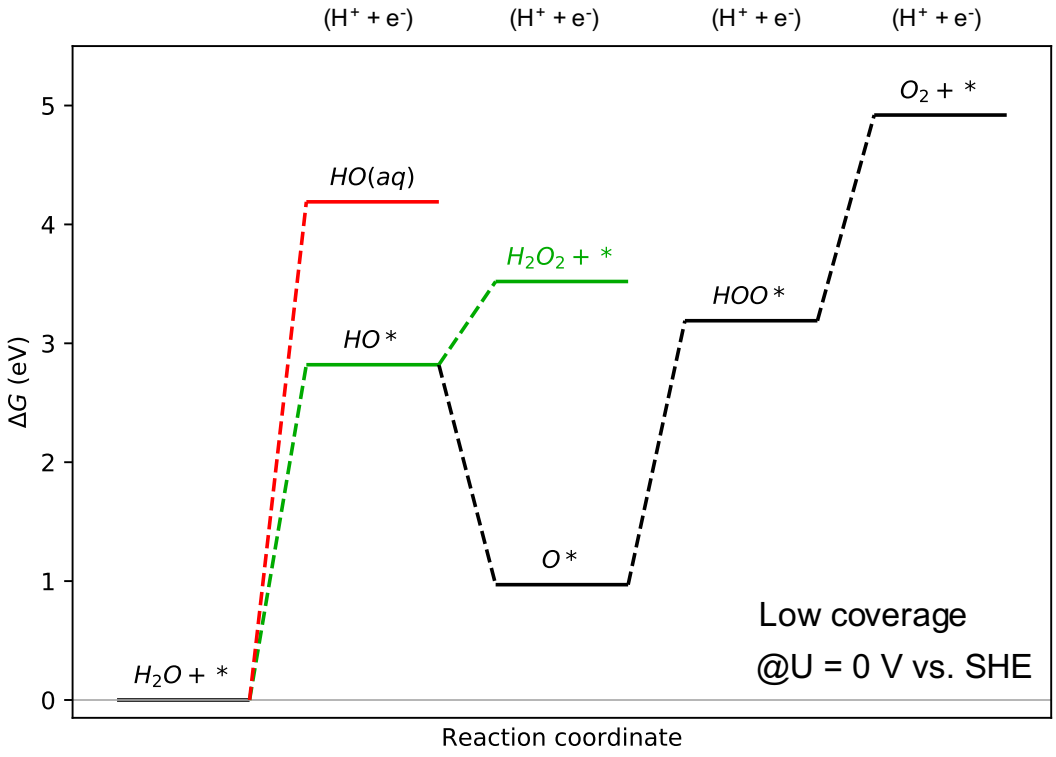


Figure S3. Free-energy diagram of the WOR generalized for graphene-like surface at zero potential @$U = 0$ V *vs*. SHE. Red, green, and black lines represent the 1 e^-, 2 e^-, and 4 e^- WOR, respectively.

Water chemisorption with subsequent HO* formation reveals ΔG_{HO*} in the range of 2.66 – 2.87 eV, in which the adsorption energies inversely correlate with the coverage. The desorption free energy of HO*, calculated as a process without e^- transfer, is 4.19 eV. This value does not depend on the catalyst surface due to the definition of the 1 e^- WOR mechanism.

For graphene, the $HO_{(aq)}$ desorption free energy is positive and exceeds the free energy of HO* adsorption. Therefore, the HO*-covered surface is more likely to exist than the pristine surface.

Graphene systems with adsorbed O* turned out to be more stable and favorable in free energy than HO*-covered surfaces, $\Delta G_{O*} < \Delta G_{HO*}$. ΔG_{O*} is in the range of 0.87 – 1.16 eV. Catalyst active surface coverage with O* is known as oxidized graphene or graphene oxide (stable electrode material). In contrast, the formation of the HOO* intermediate requires most energy to occur. This implies that graphene is not the active phase under reaction conditions, but rather the O*-covered graphene termination catalyzes the 4 e^- WOR. This is in agreement with a recent experimental study, reporting that pristine graphene-electrode surfaces are less stable than graphene oxides under anodic potential conditions.[5]

For the OER at $@U$ = 0 V *vs*. SHE, all reaction steps have positive ΔG_* values. Inclusion of the applied electrode potential is achieved by the formalism of the computational hydrogen electrode (CHE); that is, $\Delta G_* = \Delta G_*^0 - n \times e \times U$. As the electrode potential increases, the free energies of some intermediates become negative in free energy, while others may remain positive.

The free-energy landscape is displayed on **Figure S4** at the equilibrium potential for the 4 e^- WOR ($@U$ = 1.23 V *vs*. SHE). It turns out that the O*-covered surface is most negative in free energy. Therefore, we assume that the O* intermediate corresponds to the active surface phase of the catalyst for the OER. Thus, the free energy of ΔG_{O*} is set to zero, $\Delta G_{O*}(@U = 1.23\ \text{V}) = 0$ eV, and the free energies of the other RIs are recalculated by adjusting their energies relative to that of ΔG_{O*}.[6] The reordered free-energy surface at the OER equilibrium potential is shown in **Figure S5**.

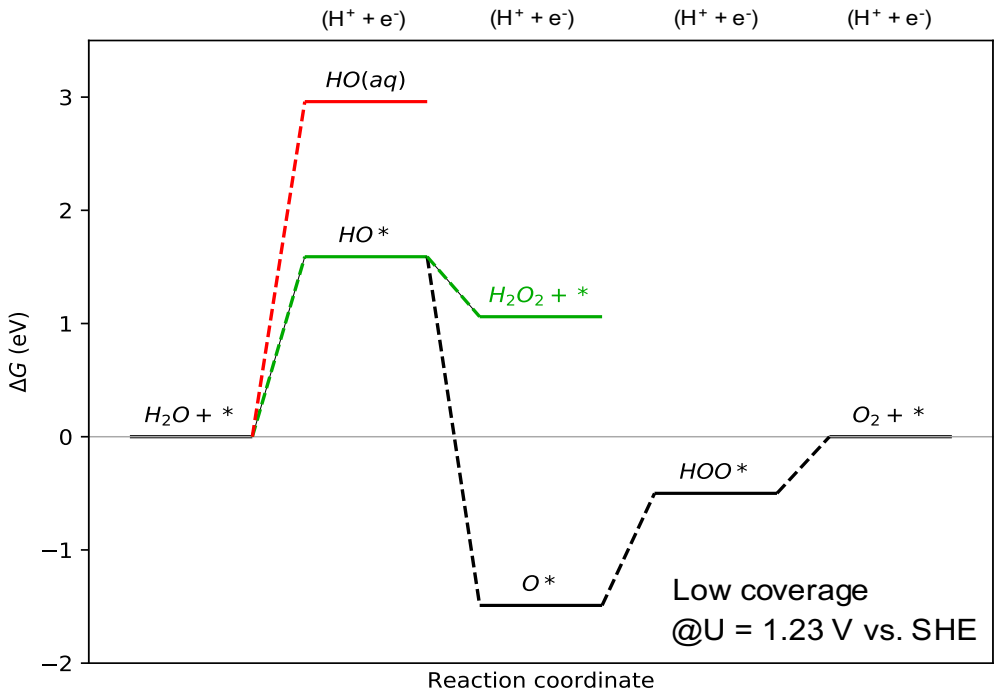


Figure S4. Free-energy diagram of the WOR generalized for graphene-like surfaces at the OER equilibrium potential (@U = 1.23 V *vs*. SHE). Red, green, and black lines represent the 1 e^-, 2 e^-, and 4 e^- WOR, respectively.

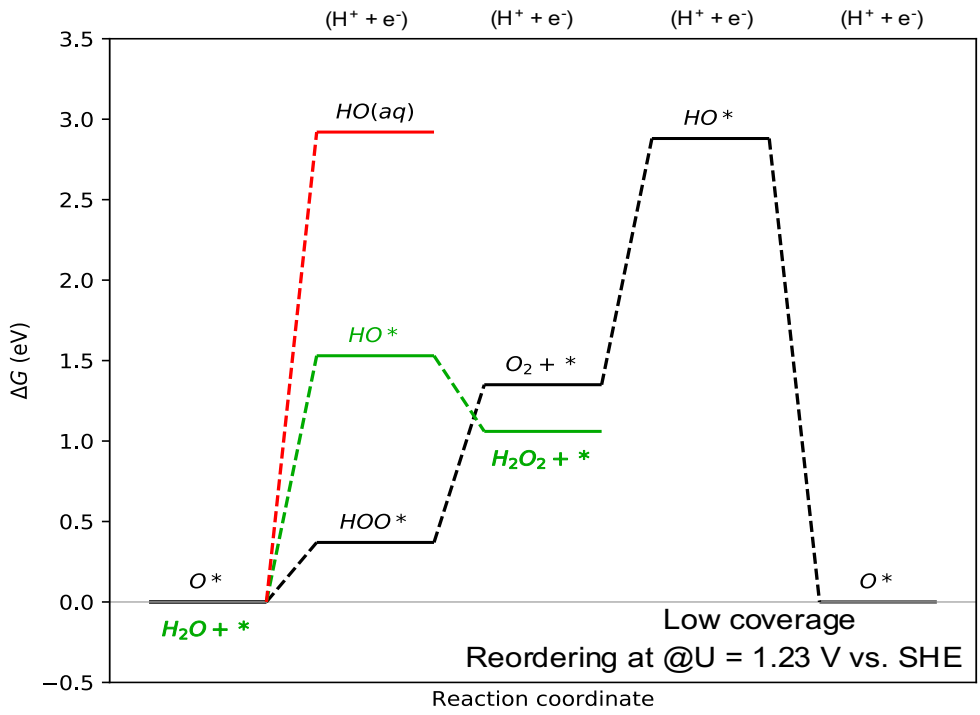


Figure S5. Free-energy diagram of the WOR at @U = 1.23 V *vs*. SHE. The elementary reaction steps of the 4 e^- WOR have been reordered, illustrating that the OER commences from the O*-covered surface.

Section 5. Selectivity and current density above the PER equilibrium potential

The free-energy diagrams in **Figure S3** and **Figure S4** depict the thermodynamics of the reactions. This may help us to identify critical reaction steps as well as to elaborate on the reaction mechanism under different values of *@U*. In this section, we describe how the PFR selectivity and PFR current density can be quantified, making use of the descriptor $G_{max}(\eta)$.[6,7]

The activity descriptor $G_{max}(\eta)$ was introduced in a recent contribution, enabling approximation of the electrocatalytic activity by advanced thermodynamic concepts:[6] $G_{max}(\eta)$ is given by the free-energy span from the intermediate with smallest free energy to the intermediate with highest free energy in the free-energy landscape; e. g., in **Figure S5**, $G_{max}(\eta = 0\ \text{V})$ corresponds to the transition from the O* to the OH* adsorbate relating to the 4 e^- WOR. Thereafter, this free-energy span is evaluated in dependence of the applied overpotential, as discussed in the main text (cf. **Figure 2**).

Since $G_{max}(\eta)$ can be quantified for the OER and PFR both, the difference between these values at a fixed electrode potential is a measure for PFR selectivity:

$$G_{sel} = G_{max}^{OER} - G_{max}^{PFR} \tag{S2}$$

Following the selectivity model of Exner for the competing chlorine and oxygen evolution reactions,[8,9] we can derive an expression for the selectivity toward the PFR from the Butler-Volmer equation:

$$PER\ sel. = \frac{exp\left(\frac{G_{sel}}{k_B T}\right)}{exp\left(\frac{G_{sel}}{k_B T}\right) + 1} \tag{S3}$$

In equation (S3), k_B is the Boltzmann constant, and T = 298.15 K. This function has values in the range between 0 (100% selectivity toward the OER) and 1 (100% selectivity toward the PFR). This measure is used in **Figure 3** in the main text for the discussion of the PFR selectivity.

The rate of an electrochemical process is governed by the rate-determining step (rds), which is described by the transition state (TS) with highest free energy in the free-energy landscape ($G^{\#}_{rds}$). It was shown that the activity descriptor $G_{max}(\eta)$ approximates $G^{\#}_{rds}$ with an offset of about 0.4 eV.[6] Therefore, we approximate $G^{\#}_{rds}$ by adding a constant of 0.4 eV to $G_{max}(\eta)$:

$$G^{\#}{}_{rds} = G^{PFR}_{max} + 0.4\ \text{eV} \tag{S4}$$

The knowledge of $G^{\#}_{rds}$ enables calculating the current density by making use of the formula:[10]

$$j \approx \frac{k_B T z e \Gamma_{act}}{h} \cdot exp\left(\frac{-G^{\#}{}_{rds}}{k_B T}\right) \tag{S5}$$

In equation (S5), z is the number of transferred electrons (2 for the PER), h is the Planck constant, and Γ_{act} is the number of active sites per unit cell's surface area. Equation (S5) is used for the calculation of the PFR current densities in **Figure 3** of the main text. Γ_{act} is inversely proportional to the surface area of the unit cell S_{cell}, and is expressed in cm^{-2}. Γ_{act} is calculated according to equation (S6), where A and B and sin (γ) are optimized parameters of the graphene unit cell.

$$\Gamma_{act} = \frac{1}{S_{cell}} = \frac{1}{A \cdot B \cdot sin\,(\gamma)} \tag{S6}$$

Section 6. Input geometries (XYZ)

SLAB4

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
0.488810246000E+01	0.000000000000E+00	0.000000000000E+00
-0.122202561500E+01	0.211661045333E+01	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	0.500000000000E+03

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02

SLAB4+O

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888102460000E+00	0.000000000000E+00	0.000000000000E+00
-1.222025615000E+00	2.116610453330E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
O	6.000000000000E-01	3.500000000000E-01	1.500000000000E+00

SLAB4+OH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888102460000E+00	0.000000000000E+00	0.000000000000E+00
-1.222025615000E+00	2.116610453330E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
O	0.000000000000E+00	0.000000000000E+00	1.500000000000E+00
H	0.000000000000E+00	6.000000000000E-01	1.800000000000E+00

SLAB4+OOH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888102460000E+00	0.000000000000E+00	0.000000000000E+00
-1.222025615000E+00	2.116610453330E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
O	1.222050000000E+00	7.055500000000E-01	1.400000000000E+00
O	1.322050000000E+00	1.805550000000E+00	2.600000000000E+00
H	1.522050000000E+00	2.005550000000E+00	3.400000000000E+00

SLAB6

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
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-3.666076845000E+00	6.349831359990E+00	0.000000000000E+00

0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.175009441523E-16	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02

SLAB6+O

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
2.444051230000E+00	0.000000000000E+00	0.000000000000E+00
-3.666076845000E+00	6.349831359990E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.175009441523E-16	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
O	7.800000000000E-01	3.900000000000E-01	1.000000000000E+00

SLAB6+OH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
2.444051230000E+00	0.000000000000E+00	0.000000000000E+00
-3.666076845000E+00	6.349831359990E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.175009441523E-16	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
O	-1.220000000000E+00	7.000000000000E-01	1.800000000000E+00
H	5.000000000000E-01	7.000000000000E-01	2.200000000000E+00

SLAB6+OOH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
2.444051230000E+00	0.000000000000E+00	0.000000000000E+00
-3.666076845000E+00	6.349831359990E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.175009441523E-16	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
O	-1.220000000000E+00	7.000000000000E-01	1.800000000000E+00
O	-1.900000000000E+00	2.000000000000E+00	2.200000000000E+00
H	-2.700000000000E+00	2.000000000000E+00	2.700000000000E+00

SLAB8

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888102460000E+00	0.000000000000E+00	0.000000000000E+00
-2.444051230000E+00	4.233220906660E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	0.000000000000E+00	-1.411073635554E+00	1.697500000000E-02
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02

SLAB8+O

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888172507460E+00	0.000000000000E+00	0.000000000000E+00
-2.444086253730E+00	4.233281569540E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.175009441523E-16	-1.411099349581E+00	-1.424103300000E-05
C	-1.222047884000E+00	7.055496747905E-01	-1.424103300000E-05
C	2.444086253730E+00	-1.411093856513E+00	-1.116134300000E-05
C	1.222047884000E+00	7.055496747905E-01	-1.424103300000E-05
C	0.000000000000E+00	0.000000000000E+00	1.691625300000E-05
C	-1.222047868669E+00	2.116638047089E+00	1.232272900000E-05
C	2.444086253729E+00	5.475363475060E-06	1.232272900000E-05
C	1.222047868670E+00	2.116638047088E+00	1.232272900000E-05
O	2.077473315670E+00	1.481648549339E+00	1.500000000000E+00

SLAB8+OH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888172507460E+00	0.000000000000E+00	0.000000000000E+00

-2.444086253730E+00	4.233281569540E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.175009441523E-16	-1.411099349581E+00	-1.424103300000E-05
C	-1.222047884000E+00	7.055496747905E-01	-1.424103300000E-05
C	2.444086253730E+00	-1.411093856513E+00	-1.116134300000E-05
C	1.222047884000E+00	7.055496747905E-01	-1.424103300000E-05
C	0.000000000000E+00	0.000000000000E+00	1.691625300000E-05
C	-1.222047868669E+00	2.116638047089E+00	1.232272900000E-05
C	2.444086253729E+00	5.475363475060E-06	1.232272900000E-05
C	1.222047868670E+00	2.116638047088E+00	1.232272900000E-05
O	4.249166156422E+00	2.986791811389E+00	1.400000000000E+00
H	4.249166156422E+00	2.986791811389E+00	2.300000000000E+00

SLAB8+OOH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888172507460E+00	0.000000000000E+00	0.000000000000E+00
-2.444086253730E+00	4.233281569540E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.175009441523E-16	-1.411099349581E+00	-1.424103300000E-05
C	-1.222047884000E+00	7.055496747905E-01	-1.424103300000E-05
C	2.444086253730E+00	-1.411093856513E+00	-1.116134300000E-05
C	1.222047884000E+00	7.055496747905E-01	-1.424103300000E-05
C	0.000000000000E+00	0.000000000000E+00	1.691625300000E-05
C	-1.222047868669E+00	2.116638047089E+00	1.232272900000E-05
C	2.444086253729E+00	5.475363475060E-06	1.232272900000E-05
C	1.222047868670E+00	2.116638047088E+00	1.232272900000E-05
O	1.222050000000E+00	7.055500000000E-01	1.400000000000E+00
O	1.322050000000E+00	1.805550000000E+00	2.600000000000E+00
H	1.522050000000E+00	2.005550000000E+00	3.400000000000E+00

SLAB12

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888102460000E+00	0.000000000000E+00	0.000000000000E+00
-3.666076845000E+00	6.349831359990E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.175009441523E-16	-1.411073635554E+00	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	2.350018883046E-16	2.822147271107E+00	1.697500000000E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02

C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	3.666076845000E+00	-2.116610453331E+00	-1.697500000000E-02

SLAB12+O

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888102460000E+00	0.000000000000E+00	0.000000000000E+00
-3.666076845000E+00	6.349831359990E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.175009441523E-16	-1.411073635554E+00	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	2.350018883046E-16	2.822147271107E+00	1.697500000000E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	3.666076845000E+00	-2.116610453331E+00	-1.697500000000E-02
O	6.000000000000E-01	3.500000000000E-01	1.600000000000E+00

SLAB12+OH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888102460000E+00	0.000000000000E+00	0.000000000000E+00
-3.666076845000E+00	6.349831359990E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.175009441523E-16	-1.411073635554E+00	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	2.350018883046E-16	2.822147271107E+00	1.697500000000E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	3.666076845000E+00	-2.116610453331E+00	-1.697500000000E-02
O	0.000000000000E+00	0.000000000000E+00	2.500000000000E+00
H	0.000000000000E+00	6.000000000000E-01	3.200000000000E+00

SLAB12+OOH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888102460000E+00	0.000000000000E+00	0.000000000000E+00
-3.666076845000E+00	6.349831359990E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.175009441523E-16	-1.411073635554E+00	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	2.350018883046E-16	2.822147271107E+00	1.697500000000E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	3.666076845000E+00	-2.116610453331E+00	-1.697500000000E-02
O	0.000000000000E+00	0.000000000000E+00	1.700000000000E+00
O	0.000000000000E+00	9.500000000000E-01	2.500000000000E+00
H	0.000000000000E+00	1.000000000000E+00	3.300000000000E+00

SLAB16

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888102460000E+00	0.000000000000E+00	0.000000000000E+00
-4.888102460000E+00	8.466441813320E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.222025615000E+00	-3.527684088884E+00	1.697500000000E-02
C	5.875047207615E-16	-1.411073635554E+00	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	4.700037766092E-16	2.822147271107E+00	1.697500000000E-02
C	3.666076845000E+00	-3.527684088884E+00	1.697500000000E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	-2.444051230000E+00	4.233220906661E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	0.000000000000E+00	4.233220906661E+00	-1.697500000000E-02
C	3.666076845000E+00	-2.116610453331E+00	-1.697500000000E-02

SLAB16+O

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888102460000E+00	0.000000000000E+00	0.000000000000E+00
-4.888102460000E+00	8.466441813320E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.222025615000E+00	-3.527684088884E+00	1.697500000000E-02
C	5.875047207615E-16	-1.411073635554E+00	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	4.700037766092E-16	2.822147271107E+00	1.697500000000E-02
C	3.666076845000E+00	-3.527684088884E+00	1.697500000000E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	-2.444051230000E+00	4.233220906661E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	0.000000000000E+00	4.233220906661E+00	-1.697500000000E-02
C	3.666076845000E+00	-2.116610453331E+00	-1.697500000000E-02
O	7.800000000000E-01	3.900000000000E-01	1.000000000000E+00

SLAB16+OH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888102460000E+00	0.000000000000E+00	0.000000000000E+00
-4.888102460000E+00	8.466441813320E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.222025615000E+00	-3.527684088884E+00	1.697500000000E-02
C	5.875047207615E-16	-1.411073635554E+00	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	4.700037766092E-16	2.822147271107E+00	1.697500000000E-02
C	3.666076845000E+00	-3.527684088884E+00	1.697500000000E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	-2.444051230000E+00	4.233220906661E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	0.000000000000E+00	4.233220906661E+00	-1.697500000000E-02
C	3.666076845000E+00	-2.116610453331E+00	-1.697500000000E-02

O	0.000000000000E+00	0.000000000000E+00	2.300000000000E+00
H	0.000000000000E+00	6.000000000000E-01	3.000000000000E+00

SLAB16+OOH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
4.888102460000E+00	0.000000000000E+00	0.000000000000E+00
-4.888102460000E+00	8.466441813320E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.222025615000E+00	-3.527684088884E+00	1.697500000000E-02
C	5.875047207615E-16	-1.411073635554E+00	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	4.700037766092E-16	2.822147271107E+00	1.697500000000E-02
C	3.666076845000E+00	-3.527684088884E+00	1.697500000000E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	-2.444051230000E+00	4.233220906661E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	0.000000000000E+00	4.233220906661E+00	-1.697500000000E-02
C	3.666076845000E+00	-2.116610453331E+00	-1.697500000000E-02
O	0.000000000000E+00	0.000000000000E+00	1.600000000000E+00
O	0.000000000000E+00	9.000000000000E-01	2.100000000000E+00
H	0.000000000000E+00	1.000000000000E+00	2.900000000000E+00

SLAB24

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
7.332153690000E+00	0.000000000000E+00	0.000000000000E+00
-4.888102460000E+00	8.466441813320E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.222025615000E+00	-3.527684088884E+00	1.697500000000E-02
C	-5.875047207615E-16	-1.411073635554E+00	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	2.350018883046E-16	2.822147271107E+00	1.697500000000E-02
C	3.666076845000E+00	-3.527684088884E+00	1.697500000000E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	-3.666076845000E+00	7.055368177769E-01	1.697500000000E-02
C	-4.888102460000E+00	2.822147271107E+00	1.697500000000E-02
C	-1.222025615000E+00	-3.527684088884E+00	1.697500000000E-02

C	-2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	-2.444051230000E+00	4.233220906661E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	4.700037766092E-16	4.233220906661E+00	-1.697500000000E-02
C	3.666076845000E+00	-2.116610453331E+00	-1.697500000000E-02
C	-2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	-3.666076845000E+00	2.116610453331E+00	-1.697500000000E-02
C	-4.888102460000E+00	4.233220906661E+00	-1.697500000000E-02
C	-1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02

SLAB24+O

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
7.332153690000E+00	0.000000000000E+00	0.000000000000E+00
-4.888102460000E+00	8.466441813320E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.222025615000E+00	-3.527684088884E+00	1.697500000000E-02
C	-5.875047207615E-16	-1.411073635554E+00	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	2.350018883046E-16	2.822147271107E+00	1.697500000000E-02
C	3.666076845000E+00	-3.527684088884E+00	1.697500000000E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	-3.666076845000E+00	7.055368177769E-01	1.697500000000E-02
C	-4.888102460000E+00	2.822147271107E+00	1.697500000000E-02
C	-1.222025615000E+00	-3.527684088884E+00	1.697500000000E-02
C	-2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	-2.444051230000E+00	4.233220906661E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	4.700037766092E-16	4.233220906661E+00	-1.697500000000E-02
C	3.666076845000E+00	-2.116610453331E+00	-1.697500000000E-02
C	-2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	-3.666076845000E+00	2.116610453331E+00	-1.697500000000E-02
C	-4.888102460000E+00	4.233220906661E+00	-1.697500000000E-02
C	-1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
O	-6.000000000000E-01	3.500000000000E-01	2.500000000000E+00

SLAB24+OH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
7.332153690000E+00	0.000000000000E+00	0.000000000000E+00
-4.888102460000E+00	8.466441813320E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.222025615000E+00	-3.527684088884E+00	1.697500000000E-02
C	-5.875047207615E-16	-1.411073635554E+00	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	2.350018883046E-16	2.822147271107E+00	1.697500000000E-02
C	3.666076845000E+00	-3.527684088884E+00	1.697500000000E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	-3.666076845000E+00	7.055368177769E-01	1.697500000000E-02
C	-4.888102460000E+00	2.822147271107E+00	1.697500000000E-02
C	-1.222025615000E+00	-3.527684088884E+00	1.697500000000E-02
C	-2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	-2.444051230000E+00	4.233220906661E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	4.700037766092E-16	4.233220906661E+00	-1.697500000000E-02
C	3.666076845000E+00	-2.116610453331E+00	-1.697500000000E-02
C	-2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	-3.666076845000E+00	2.116610453331E+00	-1.697500000000E-02
C	-4.888102460000E+00	4.233220906661E+00	-1.697500000000E-02
C	-1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
O	0.000000000000E+00	0.000000000000E+00	2.500000000000E+00
H	0.000000000000E+00	6.000000000000E-01	3.200000000000E+00

SLAB24+OOH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
7.332153690000E+00	0.000000000000E+00	0.000000000000E+00
-4.888102460000E+00	8.466441813320E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	-1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000000E-02
C	1.222025615000E+00	-3.527684088884E+00	1.697500000000E-02
C	-5.875047207615E-16	-1.411073635554E+00	1.697500000000E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000000E-02
C	2.350018883046E-16	2.822147271107E+00	1.697500000000E-02
C	3.666076845000E+00	-3.527684088884E+00	1.697500000000E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	-3.666076845000E+00	7.055368177769E-01	1.697500000000E-02

C	-4.888102460000E+00	2.822147271107E+00	1.697500000000E-02
C	-1.222025615000E+00	-3.527684088884E+00	1.697500000000E-02
C	-2.444051230000E+00	-1.411073635554E+00	1.697500000000E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000000E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	-2.444051230000E+00	4.233220906661E+00	-1.697500000000E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
C	2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000000E-02
C	4.700037766092E-16	4.233220906661E+00	-1.697500000000E-02
C	3.666076845000E+00	-2.116610453331E+00	-1.697500000000E-02
C	-2.444051230000E+00	0.000000000000E+00	-1.697500000000E-02
C	-3.666076845000E+00	2.116610453331E+00	-1.697500000000E-02
C	-4.888102460000E+00	4.233220906661E+00	-1.697500000000E-02
C	-1.222025615000E+00	-2.116610453331E+00	-1.697500000000E-02
O	0.000000000000E+00	0.000000000000E+00	3.100000000000E+00
O	0.000000000000E+00	9.500000000000E-01	3.800000000000E+00
H	0.000000000000E+00	1.000000000000E+00	4.600000000000E+00

SLAB32

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
9.776204920000E+00	0.000000000000E+00	0.000000000000E+00
-4.888102460000E+00	8.466441813320E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	0.000000000000E+00	-1.411073635554E+00	1.697500000001E-02
C	-1.222025615000E+00	7.055368177769E-01	1.697500000001E-02
C	-2.444051230000E+00	2.822147271107E+00	1.697500000001E-02
C	1.222025615000E+00	-3.527684088884E+00	1.697500000001E-02
C	2.444051230000E+00	-1.411073635554E+00	1.697500000001E-02
C	1.222025615000E+00	7.055368177769E-01	1.697500000001E-02
C	2.350018883046E-16	2.822147271107E+00	1.697500000001E-02
C	3.666076845000E+00	-3.527684088884E+00	1.697500000001E-02
C	4.888102460000E+00	-1.411073635554E+00	1.697500000001E-02
C	3.666076845000E+00	7.055368177769E-01	1.697500000001E-02
C	2.444051230000E+00	2.822147271107E+00	1.697500000001E-02
C	6.110128075000E+00	-3.527684088884E+00	1.697500000001E-02
C	-2.444051230000E+00	-1.411073635554E+00	1.697500000001E-02
C	-3.666076845000E+00	7.055368177769E-01	1.697500000001E-02
C	-4.888102460000E+00	2.822147271107E+00	1.697500000001E-02
C	-1.222025615000E+00	-3.527684088884E+00	1.697500000001E-02
C	0.000000000000E+00	0.000000000000E+00	-1.697500000001E-02
C	-1.222025615000E+00	2.116610453331E+00	-1.697500000001E-02
C	-2.444051230000E+00	4.233220906661E+00	-1.697500000001E-02
C	1.222025615000E+00	-2.116610453331E+00	-1.697500000001E-02
C	2.444051230000E+00	2.349909659450E-16	-1.697500000001E-02
C	1.222025615000E+00	2.116610453331E+00	-1.697500000001E-02
C	-4.700037766092E-16	4.233220906661E+00	-1.697500000001E-02

C	3.666076845000E+00	-2.116610453331E+00	-1.697500000001E-02
C	4.888102460000E+00	0.000000000000E+00	-1.697500000001E-02
C	3.666076845000E+00	2.116610453331E+00	-1.697500000001E-02
C	2.444051230000E+00	4.233220906661E+00	-1.697500000001E-02
C	6.110128075000E+00	-2.116610453331E+00	-1.697500000001E-02
C	-2.444051230000E+00	-1.174954829725E-16	-1.697500000001E-02
C	-3.666076845000E+00	2.116610453331E+00	-1.697500000001E-02
C	-4.888102460000E+00	4.233220906661E+00	-1.697500000001E-02
C	-1.222025615000E+00	-2.116610453331E+00	-1.697500000001E-02

SLAB32+O

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
9.776421263160E+00	0.000000000000E+00	0.000000000000E+00
-4.888210631580E+00	8.466629171990E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	0.000000000000E+00	-1.411093332065E+00	1.261752760000E-04
C	-1.222042672679E+00	7.055466660325E-01	1.261752760000E-04
C	-2.444085473300E+00	2.822210503070E+00	2.586282780000E-04
C	1.222063253835E+00	-3.527745360432E+00	2.586282780000E-04
C	2.444115511582E+00	-1.411110748542E+00	-9.778949500000E-05
C	1.222042672679E+00	7.055466660325E-01	1.261752760000E-04
C	-9.284924606915E-13	2.822221497083E+00	-9.778949500000E-05
C	3.666176784349E+00	-3.527751294655E+00	-3.750089120000E-04
C	4.888210631583E+00	-1.411126582682E+00	-3.750089120000E-04
C	3.666148727135E+00	7.055348573622E-01	2.586282780000E-04
C	2.444085473300E+00	2.822210503070E+00	2.586282780000E-04
C	6.110244478809E+00	-3.527751294653E+00	-3.750089120000E-04
C	-2.444115511581E+00	-1.411110748541E+00	-9.778949500000E-05
C	-3.666148727135E+00	7.055348573622E-01	2.586282780000E-04
C	-4.888210631580E+00	2.822209723997E+00	5.844357380000E-04
C	-1.222063253835E+00	-3.527745360432E+00	2.586282780000E-04
C	0.000000000000E+00	0.000000000000E+00	-1.332404680000E-04
C	-1.222043717411E+00	2.116654998530E+00	2.060339100000E-05
C	-2.444098199274E+00	4.233318694719E+00	4.564624200000E-05
C	1.222055141068E+00	-2.116648403078E+00	2.060339100000E-05
C	2.444098858479E+00	-6.595452438418E-06	2.060339100000E-05
C	1.222043717411E+00	2.116654998530E+00	2.060339100000E-05
C	0.000000000000E+00	4.233317703796E+00	-6.991113120000E-04
C	3.666160673776E+00	-2.116658851898E+00	-6.991113120000E-04
C	4.888210631577E+00	-8.217445455649E-06	4.564624200000E-05
C	3.666150849043E+00	2.116653179584E+00	2.912264400000E-04
C	2.444098199277E+00	4.233318694717E+00	4.564624200000E-05
C	6.110260589384E+00	-2.116658851898E+00	-6.991113120000E-04
C	-2.444098858479E+00	-6.595452438418E-06	2.060339100000E-05
C	-3.666150849042E+00	2.116653179584E+00	2.912264400000E-04
C	-4.888210631581E+00	4.233322812822E+00	2.912264400000E-04
C	-1.222055141068E+00	-2.116648403078E+00	2.060339100000E-05

O	3.900000000000E+00	1.700000000000E+00	1.200000000000E+00

SLAB32+OH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
9.776421263160E+00	0.000000000000E+00	0.000000000000E+00
-4.888210631580E+00	8.466629171990E+00	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	0.000000000000E+00	-1.411093332065E+00	1.261752760000E-04
C	-1.222042672679E+00	7.055466660325E-01	1.261752760000E-04
C	-2.444085473300E+00	2.822210503070E+00	2.586282780000E-04
C	1.222063253835E+00	-3.527745360432E+00	2.586282780000E-04
C	2.444115511582E+00	-1.411110748542E+00	-9.778949500000E-05
C	1.222042672679E+00	7.055466660325E-01	1.261752760000E-04
C	-9.284924606915E-13	2.822221497083E+00	-9.778949500000E-05
C	3.666176784349E+00	-3.527751294655E+00	-3.750089120000E-04
C	4.888210631583E+00	-1.411126582682E+00	-3.750089120000E-04
C	3.666148727135E+00	7.055348573622E-01	2.586282780000E-04
C	2.444085473300E+00	2.822210503070E+00	2.586282780000E-04
C	6.110244478809E+00	-3.527751294653E+00	-3.750089120000E-04
C	-2.444115511581E+00	-1.411110748541E+00	-9.778949500000E-05
C	-3.666148727135E+00	7.055348573622E-01	2.586282780000E-04
C	-4.888210631580E+00	2.822209723997E+00	5.844357380000E-04
C	-1.222063253835E+00	-3.527745360432E+00	2.586282780000E-04
C	0.000000000000E+00	0.000000000000E+00	-1.332404680000E-04
C	-1.222043717411E+00	2.116654998530E+00	2.060339100000E-05
C	-2.444098199274E+00	4.233318694719E+00	4.564624200000E-05
C	1.222055141068E+00	-2.116648403078E+00	2.060339100000E-05
C	2.444098858479E+00	-6.595452438418E-06	2.060339100000E-05
C	1.222043717411E+00	2.116654998530E+00	2.060339100000E-05
C	0.000000000000E+00	4.233317703796E+00	-6.991113120000E-04
C	3.666160673776E+00	-2.116658851898E+00	-6.991113120000E-04
C	4.888210631577E+00	-8.217445455649E-06	4.564624200000E-05
C	3.666150849043E+00	2.116653179584E+00	2.912264400000E-04
C	2.444098199277E+00	4.233318694717E+00	4.564624200000E-05
C	6.110260589384E+00	-2.116658851898E+00	-6.991113120000E-04
C	-2.444098858479E+00	-6.595452438418E-06	2.060339100000E-05
C	-3.666150849042E+00	2.116653179584E+00	2.912264400000E-04
C	-4.888210631581E+00	4.233322812822E+00	2.912264400000E-04
C	-1.222055141068E+00	-2.116648403078E+00	2.060339100000E-05
O	2.444056433684E+00	2.822181501899E+00	1.400000000000E+00
H	2.444056433684E+00	2.822181501899E+00	2.300000000000E+00

SLAB32+OOH

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X, Å	Y, Å	Z, Å
9.776421263160E+00	0.000000000000E+00	0.000000000000E+00
-4.888210631580E+00	8.466629171990E+00	0.000000000000E+00

0.000000000000E+00	0.000000000000E+00	5.000000000000E+02

Cartesian coordinates (primitive cell)

Atom	X, Å	Y, Å	Z, Å
C	0.000000000000E+00	-1.411093332065E+00	1.261752760000E-04
C	-1.222042672679E+00	7.055466660325E-01	1.261752760000E-04
C	-2.444085473300E+00	2.822210503070E+00	2.586282780000E-04
C	1.222063253835E+00	-3.527745360432E+00	2.586282780000E-04
C	2.444115511582E+00	-1.411110748542E+00	-9.778949500000E-05
C	1.222042672679E+00	7.055466660325E-01	1.261752760000E-04
C	-9.284924606915E-13	2.822221497083E+00	-9.778949500000E-05
C	3.666176784349E+00	-3.527751294655E+00	-3.750089120000E-04
C	4.888210631583E+00	-1.411126582682E+00	-3.750089120000E-04
C	3.666148727135E+00	7.055348573622E-01	2.586282780000E-04
C	2.444085473300E+00	2.822210503070E+00	2.586282780000E-04
C	6.110244478809E+00	-3.527751294653E+00	-3.750089120000E-04
C	-2.444115511581E+00	-1.411110748541E+00	-9.778949500000E-05
C	-3.666148727135E+00	7.055348573622E-01	2.586282780000E-04
C	-4.888210631580E+00	2.822209723997E+00	5.844357380000E-04
C	-1.222063253835E+00	-3.527745360432E+00	2.586282780000E-04
C	0.000000000000E+00	0.000000000000E+00	-1.332404680000E-04
C	-1.222043717411E+00	2.116654998530E+00	2.060339100000E-05
C	-2.444098199274E+00	4.233318694719E+00	4.564624200000E-05
C	1.222055141068E+00	-2.116648403078E+00	2.060339100000E-05
C	2.444098858479E+00	-6.595452438418E-06	2.060339100000E-05
C	1.222043717411E+00	2.116654998530E+00	2.060339100000E-05
C	0.000000000000E+00	4.233317703796E+00	-6.991113120000E-04
C	3.666160673776E+00	-2.116658851898E+00	-6.991113120000E-04
C	4.888210631577E+00	-8.217445455649E-06	4.564624200000E-05
C	3.666150849043E+00	2.116653179584E+00	2.912264400000E-04
C	2.444098199277E+00	4.233318694717E+00	4.564624200000E-05
C	6.110260589384E+00	-2.116658851898E+00	-6.991113120000E-04
C	-2.444098858479E+00	-6.595452438418E-06	2.060339100000E-05
C	-3.666150849042E+00	2.116653179584E+00	2.912264400000E-04
C	-4.888210631581E+00	4.233322812822E+00	2.912264400000E-04
C	-1.222055141068E+00	-2.116648403078E+00	2.060339100000E-05
O	2.444056433684E+00	2.822181501899E+00	1.400000000000E+00
O	2.590702752631E+00	2.568182626740E+00	2.500000000000E+00
H	2.444056433684E+00	2.822181501899E+00	3.300000000000E+00

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