Electronic Supplementary Information (ESI) for:

Reactivity at the $Cu_2O(100)$:Cu-H_2O Interface: A Combined DFT and PES study

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Contents

S1. Crystal structure and molecular optimization

1.1. The Cu_2O Crystal structure

Bulk Cu_2O adopts a cubic unit cell belonging to the *Pn3* space group. The Cu_2O structure may be described as constructed by a *face centered cubic* (fcc) Cu subblatice and a *body centered cubic* (bcc) O sublattice, or, alternatively, as two intercalated fcc Cu_2O cristobalite-like sublattices. The initial crystal structure of Cu_2O was obtained from Werner et al,[1] with an experimental lattice constant of 4.27 Å. In order to find the converged cell parameters for the unit cell at the PBE-D3+U[2–5] level of theory used in this study, different cell volumes were first tested at a 0.01 Å discretization from 4.20 to 4.40 Å without allowing for cell relaxation in VASP.[6–10] Amongst these, 4.32 Å was identified to correspond to the lowest bulk energy. From the 4.32 Å cell, a lattice relaxation was performed. This yielded the optimized lattice constant of 4.316 Å. During the optimizations, a K-point mesh of 8×8×8 and a plane-wave cut-off of 400 eV were used.

1.2. Gas phase optimization of H_2O and H_2

The molecular gas phase calculations where performed in a cubic cell of 15Å×15Å×15Å, using a single (Γ) K-point. Otherwise similar computational parameters where applied as for the surface-adsorbate calculations.

S2. Thermochemical analysis

The gas-phase molecules were treated by standard molecular thermodynamics and include contributions from the 3 translational, 3N-6 vibrational, and 3 rotational degrees of freedom as well as electronic contributions. For the surface structures, only contributions from the 3N-3 optical vibrational degrees of freedom were included in the thermochemical analysis. In other

words, the 3 low-frequency acoustic branches were not included and hence assumed to only vary moderately from structure to structure. The purpose of removing the acoustic vibrations was partly to reduce computational cost. This since acoustic vibrations are not accessible from calculations on small unit cells (as those used in this and most periodic surface–adsorbate studies), but typically demand repeating units many times larger than those used in the present study.

The thermochemical analysis was carried out assuming the ideal gas, rigid rotor and harmonic oscillator approximations, where applicable. All thermodynamic quantities were evaluated based on standard relationships as described in, e.g., ref 11.

2.1. The Partial Hessian

Below follows a short account of the producers to determine the vibrational frequencies for the surface-adsorbate states. Due to computational constraints, only a partial Hessian, $\boldsymbol{H}$, of the surface-adsorbate systems were considered. These were obtained numerically by displacing the atoms of the adsorbate and the top two Cu_2O layers ±0.015 Å in the spatial coordinates using VASP[6–10] and the PBE-D3[2–4] functional (at structures optimized at the same level of theory). The use of partial Hessians has been shown to be a reasonable approximation for Cu_2O surfaces,[12] but generally only so if one is interested in *relative* energies and not of *absolute* energies. A mass-weighted Hessian, $\boldsymbol{H}_{MW}$, as obtained from the VASP output, was used in the following analysis

2.2. Separation of acoustic and optical vibrational modes

The partial, and mass-weighted, Hessian $\boldsymbol{H}_{MW}$ from above contains contributions from both the optical modes and the translational acoustic modes (transverse, longitudinal and out-of-plane).[13]

The acoustic modes can be separated out from the $\boldsymbol{H}_{\mathrm{MW}}$. This will generate three frequencies close to 0, and 3N-3 non-zero frequencies. The separation proceeds by transformation of the $\boldsymbol{H}_{\mathrm{MW}}$ into internal coordinates by:

$$\boldsymbol{H}_{int} = \boldsymbol{D}^{\dagger}\boldsymbol{H}_{MW}\boldsymbol{D} \ ,$$

where the transformation matrix $\boldsymbol{D}$ is the defined as the matrix that converts $\boldsymbol{q}_{\mathrm{MW}}$ into the internal coordinates $\boldsymbol{q}_{\mathrm{int}}$. $\boldsymbol{D}$ is formed by:[14]

$$\boldsymbol{D} = \boldsymbol{I} - \boldsymbol{d}_1^t\boldsymbol{d}_1 - \boldsymbol{d}_2^t\boldsymbol{d}_2 - \boldsymbol{d}_3^t\boldsymbol{d}_3$$

where the vector $\boldsymbol{d}_1$, $\boldsymbol{d}_2$ and $\boldsymbol{d}_3$ are the mass-weighted and normalized translational vectors:

$$\boldsymbol{d'}_1 = \left[\sqrt{m_1}\ 0\ 0\ \sqrt{m_2}\ 0\ 0\ \cdots \sqrt{m_N}\ 0\ 0\right]$$

$$\boldsymbol{d'}_2 = \left[\ 0\ \sqrt{m_1}\ 0\ 0\ \sqrt{m_2}\ 0\ \cdots\ 0\ \sqrt{m_N}\ 0\ \right]$$

$$\boldsymbol{d'}_3 = \left[\ 0\ 0\ \sqrt{m_1}\ \ 0\ 0\ \sqrt{m_2}\ \cdots\ 0\ 0\ \sqrt{m_N}\ \right]$$

$$\boldsymbol{d}_i = \frac{1}{\|\boldsymbol{d'}_i\|}[\boldsymbol{d'}_i]$$

The vibrational frequencies can thereafter be obtained by diagonalizing $\boldsymbol{H}_{\mathrm{int}}$ and converting the resulting eigenvalues λ_{i} to frequencies, ν_{i}, by (c is the speed of light):

$$\upsilon_i = \frac{\sqrt{\lambda_i}}{2\pi c}$$

In our analysis, and after removing the acoustic modes, all vibrational frequencies below 100 cm^{-1} are set to 100 cm^{-1} in accordance with the recommendations of Cramer and co-workers for H-bonded systems.[15]

2.3.Conversion between standard states

The Gibbs free energy, G, of a system is given by:

$$G = H - TS$$

At equilibrium, the equilibrium constant K for a process/reaction relates to the standard Gibbs free energy, ΔG°, by

$$\Delta G^\circ = -RT\ln(K)$$

Assuming the study of an adsorption reaction, $H_2O(g) + S \rightarrow H_2O\text{-}S$ (S=surface) and an initial standard state of 1 bar H_2O, the above relation yields the conversion factor $\Delta\Delta G^{\circ\rightarrow *}$ to an arbitrary H_2O pressure p_{H2O}:

$$\Delta\Delta G^{\circ\rightarrow *} = -RT\ln\left(p_{H_2O}\right)$$

A similar relation is obtained for the conversion to an arbitrary H_2 pressure. The reaction Gibbs free energy for the new reference state, ΔG^*, is obtained by adding $\Delta\Delta G^{\circ\rightarrow *}$ to the standard Gibbs free reaction energy ΔG°

$$\Delta G^* = \Delta G^\circ + \Delta\Delta G^{\circ\rightarrow *}$$

In order to convert to an aqueous state the conversion factor is, assuming a H_2O concentration of 55 M (0.041 is the concentration of 1 bar of gaseous H_2O):

$$\Delta\Delta G^{\circ\rightarrow *} = -RT\ln\left(\frac{0.041}{55}\right)$$

Note that the electronic energy, E_{el}, for H_2O must be updated from $H_2O(g)$ to $H_2O(aq)$ by inclusion of solvation effects. We have done so by adding standard PCM[16,17] corrections from Gaussian09[18] calculations on monomer H_2O. Since Cramer and co-workers[15] have established that gas-phase rotation/vibrations give a good approximation to aqueous conditions if converting all vibrations below 100 cm^{-1} to 100 cm^{-1}, the thermal corrections from harmonic frequencies obtained without PCM solvation were used also for the solvated systems.

S3. Tabulated data

Below are the energies from the diagrams of **Figure 7, 9** and **11** reprinted in table format.

Table S1. Energies in eV for the c(2×2) surface unit cell for the various H_2O/OH/H adsorption/dissociation states on the ridge-dimer c(2×2) reconstructed Cu_2O(100):Cu surface. Reprints from **Figure 7** in the main article.

	State[a)]	ΔE_{el}	ΔH	ΔG	ΔH	ΔH	ΔH
		PBE-D3+U	*PBE-D3+U*	*PBE-D3+U*	*PBE*	*PBE-D3*	*HSE06-D3*
1-H_2O	***0/4***	**-0.66**	**-0.60**	**-0.10**	**-0.33**	**-0.57**	**-0.59**
1-H_2O	***1/4****	**-2.19**	**-2.19**	**-1.66**	**-1.93**	**-2.09**	**-2.80**
1-H_2O	***1/4***	**-1.11**	**-1.16**	**-0.79**	**-0.98**	**-1.08**	**-1.48**
2-H_2O	*0/4*	-1.28	-1.17	-0.21	-0.82	-1.18	-1.14
2-H_2O	*1/4**	-2.80	-2.73	-1.74	-2.25	-2.61	-3.28
2-H_2O	*2/4**	-0.55	-0.64	0.40	-0.37	-0.81	-0.46
2-H_2O	*1/4*	-1.81	-1.79	-0.95	-1.41	-1.68	-2.04
2-H_2O	*2/4*	-2.27	-2.38	-1.68	-1.98	-2.20	-3.01
3-H_2O	***0/4***	**-2.36**	**-2.16**	**-0.71**	**-1.55**	**-2.15**	**-2.26**
3-H_2O	***1/4****	**-3.57**	**-3.42**	**-1.99**	**-2.72**	**-3.28**	**-4.00**
3-H_2O	***1/4***	**-2.78**	**-2.69**	**-1.39**	**-2.06**	**-2.56**	**-3.01**
3-H_2O	***2/4***	**-3.19**	**-3.22**	**-2.04**	**-2.62**	**-3.01**	**-3.93**
3-H_2O	***3/4***	**-1.44**	**-1.65**	**-0.60**	**-1.20**	**-1.56**	**-1.48**
4-H_2O	*0/4*	-2.83	-2.56	-0.60	-1.66	-2.52	-2.43
4-H_2O	*1/4**	-3.63	-3.45	-1.44	-2.62	-3.29	-3.87
4-H_2O	*1/4*	-2.87	-2.75	-0.92	-1.97	-2.64	-2.84
4-H_2O	*2/4*	-3.09	-3.07	-1.36	-2.30	-2.86	-3.61
4-H_2O	*3/4*	-1.76	-1.89	-0.35	-1.24	-1.84	-1.76
4-H_2O	*4/4*	-0.68	-0.98	0.43	-0.42	-0.93	0.11

[a)]Degree of dissociation, xOH per surface Cu. The asterisk (*) marks H_{ad} as dissociation product rather than H_2(g).

Table S2. Energies in eV for the p(2×2) surface unit cell compared to the c(2×2) unit cell for the various H_2O/OH/H adsorption/dissociation states on the ridge-dimer c(2×2) reconstructed Cu_2O(100):Cu surface. Reprints from **Figure 9** in the main article.

State[a)]	**Δ*H*** *p(2×2)*	**Δ*G*** *p(2×2)*	**Δ*H*** *c(2×2)*
0/8	0.00	0.00	0.00
*1/8**	-1.07	-1.03	-0.89
1/8	-0.39	-0.48	-0.20
*2/8**	-1.74	-1.62	-1.78
2/8	-0.36	-0.59	-0.40
*3/8**	0.04	0.13	(-)
3/8	-0.78	-1.20	-0.71
*4/8**	2.36	2.63	(-)
4/8	-0.97	-1.46	-1.03
5/8	0.23	-0.43	0.15
6/8	1.41	0.56	1.33
7/8	2.45	1.45	2.24
8/8	3.32	2.22	3.16

[a)]Degree of dissociation, xOH per surface Cu. The asterisk (*) marks H_{ad} as dissociation product rather than H_2(g).

Table S3. Energies in eV for bilayer (BL) and monolayer (ML) adsorption for the various H_2O/OH/H adsorption/dissociation states using the c(2×2) unit cell on the ridge-dimer c(2×2) reconstructed Cu_2O(100):Cu surface. Reprints from **Figure 11** in the main article.

State[a)]	**Δ*H*** *ML*	**Δ*G*** *BL*	**Δ*H*** *ML*	**Δ*G*** *BL*
0/4	0.00	0.00	0.00	0.00
*1/4**	-0.89	-1.03	-0.84	-1.02
1/4	-0.20	-0.48	-0.31	-0.65
2/4	-0.51	-0.77	-0.76	-1.00
3/4	0.66	0.22	0.25	-0.23
4/4	1.58	1.06	1.03	0.50

[a)]Degree of dissociation, xOH per surface Cu. The asterisk (*) marks H_{ad} as dissociation product rather than H_2(g).

S4. Humid and wet conditions

Below (**Table S4**) are the results for the free energy calculations in under different wet and humid conditions summarized.

Table S4. Gibbs free energies in eV for the c(2×2) unit cell adsorption/dissociation structures on the ridge-dimer reconstructed $Cu_2O(100)$:Cu surface converted to realistic humid and wet conditions at 298.15 K. The case of standard 1 bar H_2O partial pressure, as used in the main article, is included for comparison.

		22% RH	100% RH	1 bar	55ML
1-H_2O	***0/4***	**0.03**	**-0.01**	**-0.10**	**-0.05**[a)]
1-H_2O	***1/4****	**-1.53**	**-1.57**	**-1.66**	**-1.61**[a)]
1-H_2O	***1/4***	**-0.66**	**-0.70**	**-0.79**	**-0.74**[a)]
2-H_2O	*0/4*	0.05	-0.03	-0.21	-0.10[a)]
2-H_2O	*1/4**	-1.49	-1.57	-1.74	-1.64[a)]
2-H_2O	*2/4**	0.66	0.58	0.40	0.51[a)]
2-H_2O	*1/4*	-0.70	-0.77	-0.95	-0.85[a)]
2-H_2O	*2/4*	-1.42	-1.50	-1.68	-1.57[a)]
3-H_2O	***0/4***	**-0.32**	**-0.44**	**-0.71**	**-0.55**
3-H_2O	***1/4****	**-1.61**	**-1.72**	**-1.99**	**-1.83**
3-H_2O	***1/4***	**-1.01**	**-1.13**	**-1.39**	**-1.23**
3-H_2O	***2/4***	**-1.66**	**-1.77**	**-2.04**	**-1.88**
3-H_2O	***3/4***	**-0.21**	**-0.33**	**-0.60**	**-0.44**
4-H_2O	*0/4*	-0.09	-0.25	-0.60	-0.39
4-H_2O	*1/4**	-0.93	-1.09	-1.44	-1.23
4-H_2O	*1/4*	-0.41	-0.56	-0.92	-0.70
4-H_2O	*2/4*	-0.85	-1.01	-1.36	-1.15
4-H_2O	*3/4*	0.16	0.00	-0.35	-0.14
4-H_2O	*4/4*	0.94	0.79	0.43	0.64

[a)]Probably not applicable under the given conditions due to an assumed ML structure at the surface.

S5. Effects of variations of the hydrogen pressure

The variations in the Gibbs free energy for the different adsorption/dissociation states on the c(2×2) surface as a function of the H_2-pressure is presented in **Table S5**. Only wet conditions are considered.

Table S5. Gibbs free energies in eV for the c(2×2) unit cell adsorption/dissociation structures on the ridge-dimer reconstructed $Cu_2O(100)$:Cu surface converted to different H_2 partial pressures. Wet conditions (i.e. 55 ML H_2O) have been assumed.

		1 bar	1 mbar	531 nbar	1 fbar
1-H_2O[a]	***0/4***	**-0.05**	**-0.05**	**-0.05**	**-0.05**
1-H_2O[a]	***1/4****	**-1.61**	**-1.61**	**-1.61**	**-1.61**
1-H_2O[a]	***1/4***	**-0.55**	**-0.64**	**-0.74**	**-0.97**
2-H_2O[a]	*0/4*	-0.10	-0.10	-0.10	-0.10
2-H_2O[a]	*1/4**	-1.64	-1.64	-1.64	-1.64
2-H_2O[a]	*2/4**	0.51	0.51	0.51	0.51
2-H_2O[a]	*1/4*	-0.66	-0.75	-0.85	-1.08
2-H_2O[a]	*2/4*	-1.20	-1.38	-1.57	-2.03
3-H_2O	***0/4***	**-0.55**	**-0.55**	**-0.55**	**-0.55**
3-H_2O	***1/4****	**-1.83**	**-1.83**	**-1.83**	**-1.83**
3-H_2O	***1/4***	**-1.04**	**-1.13**	**-1.23**	**-1.46**
3-H_2O	***2/4***	**-1.51**	**-1.69**	**-1.88**	**-2.34**
3-H_2O	***3/4***	**0.12**	**-0.15**	**-0.44**	**-1.13**
4-H_2O	*0/4*	-0.39	-0.39	-0.39	-0.39
4-H_2O	*1/4**	-1.23	-1.23	-1.23	-1.23
4-H_2O	*1/4*	-0.51	-0.60	-0.70	-0.93
4-H_2O	*2/4*	-0.78	-0.96	-1.15	-1.61
4-H_2O	*3/4*	0.42	0.15	-0.14	-0.83
4-H_2O	*4/4*	1.38	1.03	0.64	-0.27

[a] Probably not applicable under the given conditions due to an assumed ML structure at the surface.

S6. Additional figures and data

Here follows additional figures and data that could not be fitted into the main article but are supporting the discussion and conclusions.

6.1. H_2O adsorption and dissociation on the (3,0;1,1) surfaces structure

Adsorption energies for single and ML water onto the (3,0;1,1) reconstructed surface is reported in **Table S6**. The different adsorption sites considered on the (3,0;1,1) surface are shown in **Figure S1**. The binding geometry for H_2O adsorption at the favored site is shown in **Figure S2** and the ML structure for the OH/H_2O ML with the $OH:H_2O$ ratio of 1:5 is shown in **Figure S3**.

Table S6. Adsorption energies in eV/H_2O for the (3,0;1,1) surfaces. Energies are given as electronic energy without thermal corrections. Adsorption sites are specified in **Figure S1**.

Surface	Site/mode	E_{ad}
(3,0;1,1)	1[a,b]	-0.24
	2[a,c]	-0.27
	3[a,c]	-0.56
	4[a,d]	-0.66
	5[c,e]	-0.42
	6[a,f]	-0.70
	7[a,g]	-0.53
	H_2O ML	-0.55
	OH/H_2O ML	-0.65

[a] H-bonds to adjacent surface oxygen. [b] Moves to bridge site between Cu1 and Cu4. [c] Stays on top site. [d] Moves to hollow site in-between Cu3, Cu4 and Cu6. [e] no H-bond. [f] Resides on the edge of Cu6, leaning out from the surface reconstruction ridge. [g] Migrates to bridge site between Cu3, and Cu5.

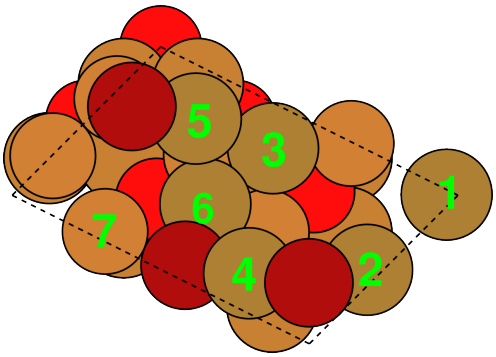

Figure S1. H_2O adsorption sites on the (3,0;1,1) surface. Note that the (2,-1;1,1) unit cell displayed here is equivalent to the (3,0;1,1) cell. Coloring: Cu_{bulk} (●), Cu_{surf} (●), O_{bulk} (●) and O_{surf} (●).

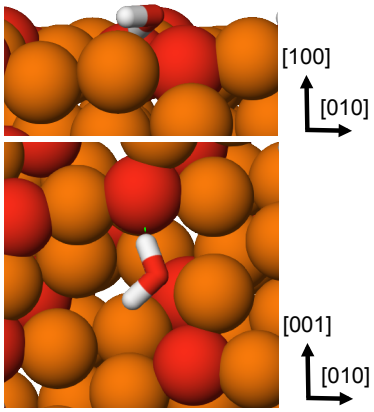

Figure S2. Water adsorption at the favored site (Cu6) on the (3,0;1,1) surface. Coloring: Cu (●), O (●) and H (○).

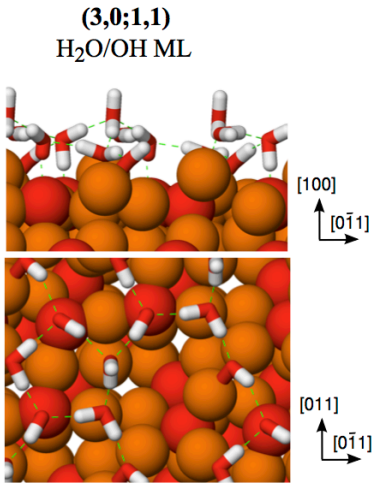

Figure S3. H_2O/OH monolayer structure on (3,0;1,1) surface. Coloring: Cu(●), O(●) and H (○).

6.2.Water interactions on the low-energy reconstructed c(2×2) surface

The adsorption energies for water onto the low-energy c(2×2) reconstructed surface are given in **Table S7**. **Figure S4** shows the various adsorption sites. Consult the main article for a discussion on the modes of water interaction on the surface.

Table S7. Adsorption energies, E_{ad}, for the different sites depicted in **Figure S4** on the low-energy reconstructed c(2×2) surface. The energies are given as electronic energies at the DFT PBE-D3+U level of theory.

Surface site[a)]	E_{ad} **[eV]**
A1	-0.38
A2	-0.51
A3	-0.72 (-0.97)[b)]
A4	-0.60
B1	-0.32
B2	-0.39
B3	-0.43
B4	-0.69
B5	-0.57
H1	-0.35
H2	-0.53
H3	-0.43

[a)] H_2O forms H-bond with the O atom on the substrate surface in all cases but B4 and H3. [b)] Obtained upon full relaxation of top two Cu_2O layers and the interacting H_2O.

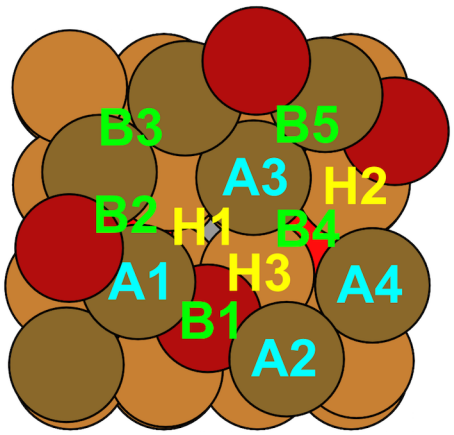

Figure S4. Depicts H_2O adsorption sites for the low-energy reconstructed c(2×2) surface. Coloring: Cu(●), O (●) and H (○).

6.3.H_2O monolayer on the ridge-dimer c(2×2) using the p(2×2) unit cell

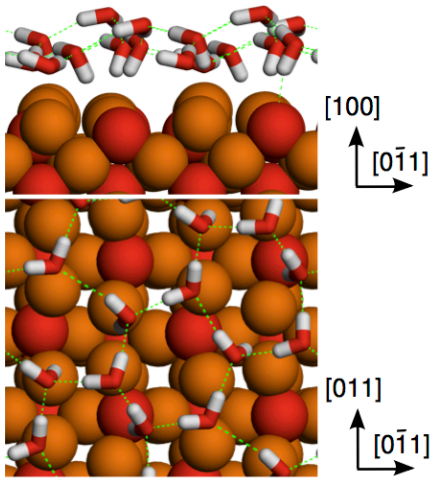

Figure S5. Shows the H_2O monolayer structure on top of the ridge dimer reconstructed c(2×2) surface using the p(2×2) unit cell.

6.4.Cooperative effects

Analysis of the H_2O adsorption processes reveal strong cooperative effects upon binding to the Cu_2O(100):Cu surface, especially at intermediate H_2O coverage and with pre-adsorbed OH. Two series were used to analyze the cooperative effect: i) adsorption to the clean ridge-dimer

reconstructed surface using a c(2×2) unit cell, and ii) adsorption to a OH/H pre-covered surface (0.125 ML OH) using a p(2×2) unit cell. These are referred to throughout the main article.

In previous study by Cox and Schulz[19] the desorption of a H_2O covered $Cu_2O(100)$:Cu surface was studied by ramping from low (110 K) to high temperatures (600 K). Our computational data can be compared to the data from Cox and Schulz (see Figure 2 in ref. 19). They found that the adsorption energy for H_2O decreases with the H_2O coverage, which indicates that the cooperative effect is largest at low coverage. The trends of Cox and Schulz are here reproduced by the DFT calculations for high water coverage on the c(2×2) unit cell (see **Figure S6** and **Figure 7** of the main article). Nevertheless, at intermediate to lower coverage the computational trend is reversed to the experimentally observed. In order to understand why computations and experiments differ, we used another approach: Since both experimental and computational results indicate H_2O dissociation on the surface, the adsorption study was repeated using a p(2×2) surface unit cell and $Cu_2(100)$:Cu-$(OH/H)_{(ad)}$ as reference state. Hence assuming 0.125 ML initial OH coverage. The experimental trend can now qualitatively be reproduced (see **Figure S6**): the adsorption energy as well as the cooperative effect are largest at low coverage, and decline as the coverage increases.

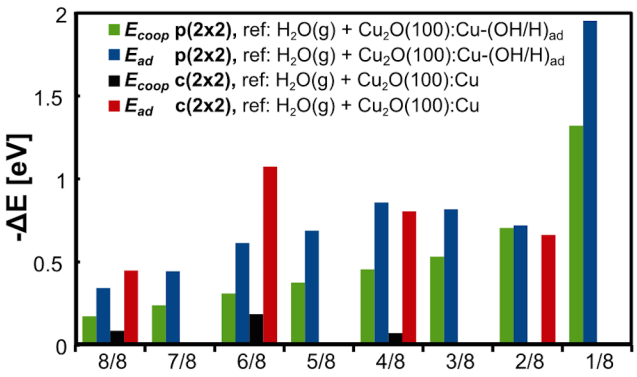

Figure S6. Sequential adsorption energies (note that no thermal corrections are added) onto bare $Cu_2O(100)$:Cu (red series) as well as onto an OH/H pre-adsorbed surface (blue). A ridge-dimer structure was assumed. The horizontal axis depicts the surface coverage. For the OH/H pre-adsorbed series, 0.125 ML coverage indicate the first dissociative adsorption, i.e. $Cu_2O(100)$:Cu + $H_2O(g)$ → $Cu_2O(100)$:Cu-$(OH/H)_{ad}$. The green and black series show the cooperative effect of co-adsorption for the bare (black) and pre-covered (green) surfaces. Note that the c(2×2) unit cell was used to represent the bare surface, hence only 0.25, 0.5, 0.75 and 1ML adsorption are included.

6.5.NBO and Mulliken partial charge analysis

Figure S7 shows the cluster model used for the computations of the natural bond orbital (NBO)[20] and Mulliken charges for the H and OH adsorbates. The cluster was cut out from the ridge-dimer surface template. Charge neutrality and conservation of Cu_2O stoichiometry were prioritized when choosing the cluster model. In order to saturate the cluster and to ensure a charge distribution similar to the periodic Cu_2O surface, dangling and unsaturated Cu and O atoms where terminated by OH and H groups respectively. The above procedure follows the recommendations of ref. 21 and 22.

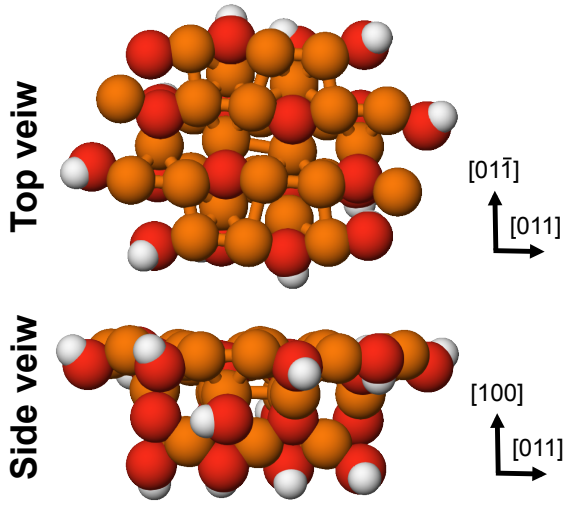

Figure S7. Shows the $(Cu_2O)_{15}$ cluster model used for the NBO and Mulliken partial charges calculations.

Initially, the cluster atoms of the clean surface where kept at there original surface positions while the terminating OH and H groups where relaxed. In the next step all atoms where constraint apart from the adsorbate and the Cu and O atoms in direct contact with the adsorbing OH and H. The OH and H groups where placed at the favored B1 position (see original article).

All cluster where optimized by DFT calculations. These where carried using the Orca program system,[23] employing the PBE0[24]-D3[3,4] xc-functional, the split-J[25] def2-SVP/J basis set[26–28] and the RIJCOSX algorithm.[29] The NBO and Mulliken charges where obtained by single point calculations at the PBE0-D3/LACV3P**++[30,31] level of theory using the Gaussian 09 program suit.[18]

S7. Convergence test for computational parameters

Table S8 summarizes the results from our convergence test for the parameters: i) the number of K-points, ii) the plane-wave cut-off and iii) the vacuum distance between two repeating slabs. **Table S9** shows a comparison of the results for the adsorption and dissociation states on the c(2×2) surface allowing the top two (2L) or top four layers (4L) to relax. Clearly the latter does not result in any large differencens from the 2L case.

Table S8. Convergecy test for critical computational parametars: i) number of K-points, ii) plane-wave cut-off and iii) vacumm distance between the model slabs. The test was conducted on water adsorption onto the ridge-dimer c(2×2) reconstructed surface. The energies are reported in eV.

K-points	$E_{ad}(H_2O)$		Cut-off	$E_{ad}(H_2O)$		Vacuum	$E_{ad}(H_2O)$
2×2×1	-0.64		*320 eV*	-0.68		*12 Å*	-0.68
4×4×1	-0.66		*400 eV*	-0.66		*17 Å*	-0.66
8×8×1	-0.66		*520 eV*	-0.66		*22 Å*	-0.66
			800 eV	-0.66		*17 Å*[a)]	-0.66

[a)] Employing dipole corrections, otherwise not.

Table S9. Electronic energy for the various surface states at the PBE-D3+U level of theory with the two or four topmost Cu_2O layers unconstraint during the geometrical relaxation.

	State	2L	4L
1-H_2O	***0/4***	**-0.66**	**-0.66**
1-H_2O	***1/4****	**-2.19**	**-2.18**
1-H_2O	***1/4***	**-1.11**	**-1.12**
2-H_2O	*0/4*	-1.28	-1.28
2-H_2O	*1/4**	-2.80	-2.79
2-H_2O	*2/4**	-0.55	-0.53
2-H_2O	*1/4*	-1.81	-1.82
2-H_2O	*2/4*	-2.27	-2.25
3-H_2O	***0/4***	**-2.36**	**-2.35**
3-H_2O	***1/4****	**-3.57**	**-3.56**
3-H_2O	***1/4***	**-2.78**	**-2.80**
3-H_2O	***2/4***	**-3.19**	**-3.17**
3-H_2O	***3/4***	**-1.44**	**-1.42**
4-H_2O	*0/4*	-2.83	-2.85
4-H_2O	*1/4**	-3.63	-3.65
4-H_2O	*1/4*	-2.87	-2.90
4-H_2O	*2/4*	-3.09	-3.07
4-H_2O	*3/4*	-1.76	-1.75
4-H_2O	*4/4*	-0.68	-0.69

S8. Experimental coverage determination from O 1s PES data

The photoelectron inelastic mean free paths for the compounds of interest in the present study were calculated using the Tanuma-Penn-Powell algorithm[32] from the NIST Electron Inelastic-Mean-Free-Path Database.[33] The photoionization cross sections are assumed to be constant for

the O 1s core level in all compounds and a normal photoelectron emission angle geometry was used in all relevant experiments. In the calculations we used a kinetic energy of 120 eV and the following compound specific parameters: band gap (E_g^{Cu2O} = 2.2 eV,[34] E_g^{H2O} = 7.0 eV[35]), density (ρ^{Cu2O} = 6 gcm^{-3},[36] ρ^{H2O} = 0.9971 gcm^{-3} [37]), and the number of valence electrons (N_v^{Cu2O} = 28, N_v^{H2O} = 8 [32]). The resulting mean free paths at 120 eV kinetic energy are λ^{Cu2O} = 5.37 Å for Cu_2O and λ^{H2O} = 8.65 Å for H_2O. The inelastic mean free path of OH was assumed to be equal to that of H_2O. The thickness of a monolayer of hydroxyl groups was defined using the DFT geometry from the present study for OH adsorbed on Cu_2O(100), 2.89 Å. The thickness of a monolayer of adsorbed water was obtained from the average thickness of a molecular layer of water in bulk liquid water, 3.1 Å, using the bulk liquid water density.[37] The calculated thicknesses of the OH and H_2O layers were converted into monolayer coverage by dividing by their respective layer thickness. The coverage of H_2O and OH was estimated from their fraction of the intensity of the integrated O 1s intensity. A layered structure was assumed in the simulations with H_2O adsorbed closest to the vacuum and OH at the Cu_2O interface. The photoelectron contributions from the H_2O and OH layers as well as from a Cu_2O slab with a thickness exceeding 10 nm was integrated after the signal from each excitation depth was subjected to exponential decay when travelling through the relevant layers to the vacuum. The coverage was estimated from an iterative procedure.

S9. Supplementary references

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S10. Appendix: Cartesian coordinates

Below are the XYZ-coordinates for the optimized adsorption and dissociation structures included. All structures have been optimized at the PBE-D3+U level of theory. The coordinates for the surface reconstruction structure without adsorbates can be obtained from the supporting info for supplementary ref. 38 (ref. 17 in main article).

10.1. Ridge-dimer c(2×2) structures - c(2×2) unit cell

Structures displayed in **Figure 8** of the main article.

0.25 ML H_2O coverage – 0/4 OH

39

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	-0.400399999999984	3.197130000000005	12.226650000000033
Cu	-0.400399999999983	1.041220000000010	10.070740000000047
Cu	-2.555589999999989	5.352320000000010	12.226650000000033
Cu	-0.400400000000014	7.507499999999993	16.538479999999911
Cu	-0.400399999999984	3.197130000000005	16.538479999999911
Cu	-0.400399999999983	1.041220000000010	14.382569999999925
Cu	1.754780000000000	3.196399999999993	10.070740000000047
Cu	-2.555589999999989	5.352320000000010	16.538479999999911
Cu	-0.400400000000015	5.351589999999998	14.382569999999925
Cu	1.754780000000000	3.196399999999993	14.382569999999925

Cu	-2.555590000000019	3.196399999999993	14.382569999999925
Cu	1.754780000000000	5.352319999999979	16.538479999999911
Cu	-0.400400000000014	7.507499999999993	12.226650000000033
Cu	-0.400400000000015	5.351589999999998	10.070740000000047
Cu	-2.555590000000019	3.196399999999993	10.070740000000047
Cu	1.754780000000000	5.352319999999979	12.226650000000033
Cu	-0.277588165946309	3.608673901671624	20.204898240818643
Cu	-0.488801487585674	0.933196250775558	18.630045275998992
Cu	-2.083278267780846	5.363424550008094	20.393675564519974
Cu	1.810016867733400	4.950975809128182	20.210769192436725
Cu	-0.836978979271115	7.544727439103029	20.202062491254537
Cu	-0.249014155252634	5.549868274501618	18.648155780805872
Cu	1.633614996214465	2.969083630624180	18.543641298602807
Cu	-2.406417760904469	3.319616784658828	18.679985432823017
O	-1.358992602308679	4.395073432423881	17.577944872574168
O	0.872260059461186	6.632533367352847	19.862434780452077
O	0.561140614510891	1.929242504570702	19.750168863934270
O	2.736515036313166	4.179523609065452	17.543659692911802
O	0.677549999999987	6.429539999999999	11.148700000000101
O	2.832739999999992	4.274359999999986	8.992779999999994
O	-1.477629999999996	4.274360000000017	13.304610000000086
O	0.677549999999987	6.429539999999999	15.460529999999977
O	2.832739999999992	4.274359999999986	13.304610000000086
O	-1.477629999999996	4.274360000000017	8.992779999999994
O	0.677550000000018	2.119170000000012	15.460529999999977
O	0.677550000000018	2.119170000000012	11.148700000000101
H	-2.978646553794381	3.250483838848620	21.394033197225642
H	-3.323051086632587	4.353909524638055	22.467060042176232
O	-2.583922578756926	3.981844035580480	21.946527656810293

0.25 ML H_2O coverage – 1/4* OH

39

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	-0.400855094987342	3.200763860731604	12.226650000000033
Cu	-0.400855094987342	1.042403451555298	10.070740000000047
Cu	-2.558494685811035	5.358403451555297	12.226650000000033
Cu	-0.400855094987373	7.516033031012959	16.538479999999911
Cu	-0.400855094987342	3.200763860731604	16.538479999999911
Cu	-0.400855094987342	1.042403451555298	14.382569999999925
Cu	1.756774484470320	3.200033031012960	10.070740000000047
Cu	-2.558494685811035	5.358403451555297	16.538479999999911
Cu	-0.400855094987373	5.357672621836652	14.382569999999925
Cu	1.756774484470320	3.200033031012960	14.382569999999925
Cu	-2.558494685811065	3.200033031012960	14.382569999999925
Cu	1.756774484470320	5.358403451555267	16.538479999999911
Cu	-0.400855094987373	7.516033031012959	12.226650000000033
Cu	-0.400855094987373	5.357672621836652	10.070740000000047
Cu	-2.558494685811065	3.200033031012960	10.070740000000047
Cu	1.756774484470320	5.358403451555267	12.226650000000033
Cu	-0.599876304834079	3.433397052380350	20.405885191726853
Cu	-0.390585414611553	1.071143277235628	18.656649851461658
Cu	-2.368663979318350	5.193403435817137	20.405719415621995
Cu	1.748684769687268	5.326490678391274	20.610919000268876
Cu	-0.482741890107295	7.562607194326104	20.607917936450246
Cu	-0.384611510280700	5.397152959658094	18.549386275616008
Cu	1.726357647592729	3.185987987598950	18.644533667352913
Cu	-2.587509332278970	3.189970522778444	18.558858298484846
O	-1.477847237948649	4.280769578655905	17.552552786144062
O	0.655856820858364	6.464056647840403	19.646984923438097
O	0.661640677411640	2.142493736900012	19.771205606557892
O	2.836017855609914	4.279968462568033	17.602585596348199
O	0.678320103917781	6.436847820741805	11.148700000000101

O	2.835959694741474	4.279218241284113	8.992779999999994
O	-1.479309475539881	4.279218241284144	13.304610000000086
O	0.678320103917781	6.436847820741805	15.460529999999977
O	2.835959694741474	4.279218241284113	13.304610000000086
O	-1.479309475539881	4.279218241284144	8.992779999999994
O	0.678320103917812	2.121578650460451	15.460529999999977
O	0.678320103917812	2.121578650460451	11.148700000000101
H	3.255813483963656	4.748436826777705	22.373397675118344
H	-1.493964635006934	4.303968553813883	21.366850713479984
O	2.732012868543550	4.225391597214492	21.738767136621963

0.25 ML H_2O coverage – 1/4 OH

38

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	-0.400855094987342	3.200763860731604	12.226650000000033
Cu	-0.400855094987342	1.042403451555298	10.070740000000047
Cu	-2.558494685811035	5.358403451555297	12.226650000000033
Cu	-0.400855094987373	7.516033031012959	16.538479999999911
Cu	-0.400855094987342	3.200763860731604	16.538479999999911
Cu	-0.400855094987342	1.042403451555298	14.382569999999925
Cu	1.756774484470320	3.200033031012960	10.070740000000047
Cu	-2.558494685811035	5.358403451555297	16.538479999999911
Cu	-0.400855094987373	5.357672621836652	14.382569999999925
Cu	1.756774484470320	3.200033031012960	14.382569999999925
Cu	-2.558494685811065	3.200033031012960	14.382569999999925
Cu	1.756774484470320	5.358403451555267	16.538479999999911
Cu	-0.400855094987373	7.516033031012959	12.226650000000033
Cu	-0.400855094987373	5.357672621836652	10.070740000000047
Cu	-2.558494685811065	3.200033031012960	10.070740000000047
Cu	1.756774484470320	5.358403451555267	12.226650000000033
Cu	-0.241574055872398	3.419138951770787	20.624738411504122
Cu	-0.524033185418446	0.922458787359075	18.681608154306446

Cu	-2.352914174333961	5.532768589426890	20.625867257952173
Cu	1.818583957077997	4.960401274046794	20.228205373614443
Cu	-0.799327522872756	7.579188577428763	20.226760902838709
Cu	-0.309767267860731	5.450221650813885	18.627085924882891
Cu	1.643046942167205	3.089715920594572	18.595142742730015
Cu	-2.529532037639916	3.230806608020881	18.669597817465089
O	-1.438836407614274	4.321029571489354	17.613373221441385
O	0.749074946381666	6.509074476416941	19.804438425186284
O	0.555666651410050	2.011277582185449	19.696277878579398
O	2.751539218914641	4.194836930882935	17.533019357239944
O	0.678320103917781	6.436847820741805	11.148700000000101
O	2.835959694741474	4.279218241284113	8.992779999999994
O	-1.479309475539881	4.279218241284144	13.304610000000086
O	0.678320103917781	6.436847820741805	15.460529999999977
O	2.835959694741474	4.279218241284113	13.304610000000086
O	-1.479309475539881	4.279218241284144	8.992779999999994
O	0.678320103917812	2.121578650460451	15.460529999999977
O	0.678320103917812	2.121578650460451	11.148700000000101
H	-0.614962572187882	5.156719955702302	22.230761639688531
O	-1.209418985918912	4.563149761048433	21.735881664045166

0.50 ML H_2O coverage – 0/4 OH

42

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	2.157994993440015	6.473994993440014	11.467750096282828
Cu	0.000000000000000	0.000000000000000	11.467750096282828
Cu	0.000000000000000	4.316000000000000	7.155909920364136
Cu	0.000000000000000	4.316000000000000	11.467750096282828
Cu	2.157994993440015	2.157994993440015	7.155909920364136
Cu	-2.158005006559985	4.316000000000000	5.000000094560074

Cu	0.000000000000000	2.157994993440015	5.000000094560074
Cu	0.000000000000000	0.000000000000000	7.155909920364136
Cu	0.000000000000000	6.473994993440015	9.311830008323588
Cu	2.157994993440015	4.316000000000000	5.000000094560074
Cu	2.157994993440015	6.473994993440014	7.155909920364136
Cu	2.157994993440015	4.316000000000000	9.311830008323588
Cu	0.000000000000000	6.473994993440015	5.000000094560074
Cu	2.157994993440015	2.157994993440015	11.467750096282828
Cu	-2.158005006559985	4.316000000000000	9.311830008323588
Cu	0.000000000000000	2.157994993440015	9.311830008323588
Cu	2.337661738904627	2.459021595010295	15.077386704690445
Cu	2.289035258720018	4.443435536269291	13.568237316682985
Cu	0.155224545794513	2.224916297746411	13.642031940405909
Cu	0.535925132901678	4.216491168298918	15.402078493564263
Cu	1.831103989161301	6.497798712905647	15.184562575599282
Cu	-2.165745591843661	4.168975107539538	13.560646994081910
Cu	-0.009367872645630	6.209266024798637	13.481244202542957
Cu	0.128161347636025	8.196226095501840	15.182710453912458
O	-1.051094810669397	5.131902956578274	14.655404583852738
O	1.166097237970811	3.319888615924115	12.520528003438951
O	-0.901615745862351	1.153347655848711	14.719976843606478
O	1.003016395558884	7.478469509103375	12.479731828436035
O	-1.079002503279992	5.395002503279992	10.389790052303100
O	-1.079002503279993	1.079002503279993	6.077960138539800
O	-1.079002503279993	1.079002503279993	10.389790052303100
O	-1.079002503279992	5.395002503279992	6.077960138539800
O	-3.236997496720007	3.236997496720007	8.233869964343864

O	1.079002503279993	3.236997496720007	8.233869964343864
O	-3.236997496720007	3.236997496720007	3.922040050580346
O	1.079002503279993	3.236997496720007	3.922040050580346
H	-0.657283679160061	3.522001477552063	17.581789905564730
H	-2.791616065746869	3.437770119430116	17.039527607366924
H	-2.620874000154799	2.801105095558100	18.456723094046367
H	0.713797959794142	2.710763402609734	17.535939421344384
O	-2.295091246821521	3.541825068987229	17.908459981179167
O	0.325784007507140	3.585812069949146	17.344785473240290

0.50 ML H_2O coverage – 1/4* OH

42

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	-0.400855094987342	3.200763860731604	12.226650000000033
Cu	-0.400855094987342	1.042403451555298	10.070740000000047
Cu	-2.558494685811035	5.358403451555297	12.226650000000033
Cu	-0.400855094987373	7.516033031012959	16.538479999999911
Cu	-0.400855094987342	3.200763860731604	16.538479999999911
Cu	-0.400855094987342	1.042403451555298	14.382569999999925
Cu	1.756774484470320	3.200033031012960	10.070740000000047
Cu	-2.558494685811035	5.358403451555297	16.538479999999911
Cu	-0.400855094987373	5.357672621836652	14.382569999999925
Cu	1.756774484470320	3.200033031012960	14.382569999999925
Cu	-2.558494685811065	3.200033031012960	14.382569999999925
Cu	1.756774484470320	5.358403451555267	16.538479999999911
Cu	-0.400855094987373	7.516033031012959	12.226650000000033
Cu	-0.400855094987373	5.357672621836652	10.070740000000047

Cu	-2.558494685811065	3.200033031012960	10.070740000000047
Cu	1.756774484470320	5.358403451555267	12.226650000000033
Cu	-0.219565048561327	3.246213099084652	20.578190203568752
Cu	-0.307575532840676	1.023134994278571	18.577286877341024
Cu	-2.299483976447037	5.290630393529744	20.595613900242583
Cu	2.084428368932711	5.106435493986814	20.531768800510847
Cu	-0.461445080461163	7.610609968547871	20.361820173436701
Cu	-0.279034953839735	5.342483777462291	18.625744877030233
Cu	1.815533385087290	3.151735694504317	18.560702910225992
Cu	-2.475332824078500	3.148620890803386	18.638335743580104
O	-1.450063549599824	4.305131714131062	17.596123397745618
O	0.832428735260745	6.355162537532248	19.727318114724341
O	0.817963061866403	2.028483137684894	19.647864162148970
O	2.860313412775966	4.304268408309031	17.550215456215483
O	0.678320103917781	6.436847820741805	11.148700000000101
O	2.835959694741474	4.279218241284113	8.992779999999994
O	-1.479309475539881	4.279218241284144	13.304610000000086
O	0.678320103917781	6.436847820741805	15.460529999999977
O	2.835959694741474	4.279218241284113	13.304610000000086
O	-1.479309475539881	4.279218241284144	8.992779999999994
O	0.678320103917812	2.121578650460451	15.460529999999977
O	0.678320103917812	2.121578650460451	11.148700000000101
H	-0.648027038325117	4.871473870934498	22.269765476861551
H	-2.223842103332592	2.855926261352728	22.481588082133470
H	2.215659304565305	5.854838568179879	23.304784206244154
H	2.997790137150038	4.130527912751840	21.369900935635432
O	-1.245015801051908	4.271219016121746	21.777400117700271

O 1.642381678390805 6.303478686365802 22.657095020812726

0.50 ML H_2O coverage – 1/4 OH

41

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu -0.400787229552186 3.200221966079347 12.226650000000033

Cu -0.400787229552186 1.042226970914926 10.070740000000047

Cu -2.558061528399799 5.357496264926960 12.226650000000033

Cu -0.400787229552186 7.514760554103477 16.538479999999911

Cu -0.400787229552186 3.200221966079347 16.538479999999911

Cu -0.400787229552186 1.042226970914926 14.382569999999925

Cu 1.756477059624332 3.199491260091444 10.070740000000047

Cu -2.558061528399799 5.357496264926960 16.538479999999911

Cu -0.400787229552186 5.356765558938994 14.382569999999925

Cu 1.756477059624332 3.199491260091444 14.382569999999925

Cu -2.558061528399768 3.199491260091412 14.382569999999925

Cu 1.756477059624332 5.357496264926960 16.538479999999911

Cu -0.400787229552186 7.514760554103477 12.226650000000033

Cu -0.400787229552186 5.356765558938994 10.070740000000047

Cu -2.558061528399768 3.199491260091412 10.070740000000047

Cu 1.756477059624332 5.357496264926960 12.226650000000033

Cu -0.495856504099471 0.940385437890393 18.705453736753697

Cu -2.276773329730047 5.486749876687553 20.612493906715461

Cu 1.975810428801598 4.962216536670228 20.440237647208701

Cu -0.657156502519249 7.558498049058132 20.212768865683376

Cu -0.278576673575352 5.366842799801194 18.625319155696729

Cu 1.706671769432988 3.171245749008750 18.653229198152221

Cu	-2.508210207385317	3.176476921984501	18.643409030802147
Cu	-0.316903520756250	3.321744215814058	20.580847136215947
O	-1.479059025982010	4.278493762509171	8.992779999999994
O	0.678205263194508	2.121219463661620	15.460529999999977
O	0.678205263194508	2.121219463661620	11.148700000000101
O	0.678205263194508	6.435758051685688	11.148700000000101
O	2.835479562042090	4.278493762509202	8.992779999999994
O	-1.479059025982010	4.278493762509171	13.304610000000086
O	0.678205263194508	6.435758051685688	15.460529999999977
O	2.835479562042090	4.278493762509202	13.304610000000086
O	-1.447998719939805	4.309344201148564	17.607996676962742
O	0.799739042565767	6.405830074411623	19.751316683876105
O	0.648053986604816	2.012646562182006	19.683856054944240
O	2.786151900628558	4.231696673674021	17.542888732657712
H	-1.720851442346315	3.979254057722014	22.405782722254386
H	0.391975961569637	5.136642639169182	22.402207735531814
H	1.724704774105325	4.710341256198630	23.124793497610707
O	1.363685822207327	5.368034055092631	22.501925380945075
O	-1.158816444168075	4.506670770249152	21.805065915202196

0.50 ML H_2O coverage – 2/4* OH

42

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	-0.400855094987342	3.200763860731604	12.226650000000033
Cu	-0.400855094987342	1.042403451555298	10.070740000000047
Cu	-2.558494685811035	5.358403451555297	12.226650000000033
Cu	-0.400855094987373	7.516033031012959	16.538479999999911

Cu	-0.400855094987342	3.200763860731604	16.538479999999911
Cu	-0.400855094987342	1.042403451555298	14.382569999999925
Cu	1.756774484470320	3.200033031012960	10.070740000000047
Cu	-2.558494685811035	5.358403451555297	16.538479999999911
Cu	-0.400855094987373	5.357672621836652	14.382569999999925
Cu	1.756774484470320	3.200033031012960	14.382569999999925
Cu	-2.558494685811065	3.200033031012960	14.382569999999925
Cu	1.756774484470320	5.358403451555267	16.538479999999911
Cu	-0.400855094987373	7.516033031012959	12.226650000000033
Cu	-0.400855094987373	5.357672621836652	10.070740000000047
Cu	-2.558494685811065	3.200033031012960	10.070740000000047
Cu	1.756774484470320	5.358403451555267	12.226650000000033
Cu	-0.138926464623378	3.424487250675960	20.794365595432890
Cu	-0.401115685156908	1.135046803983947	18.527457394220910
Cu	-2.501400816733454	5.345863902431484	20.730404626852579
Cu	1.920856433751461	5.099899846022689	20.545149169610099
Cu	-0.410233232093652	7.680690841521485	20.407703828064164
Cu	-0.378014002095055	5.317411942422906	18.606515051165307
Cu	1.773410210202563	3.211695203072716	18.660167375473950
Cu	-2.557818893620023	3.095437683299898	18.531496169676782
O	-1.495318530577254	4.267159051163565	17.583476718474209
O	0.727298809258315	6.354935347415944	19.628427560777471
O	0.677567186275528	2.112171987169183	19.666245335801449
O	2.839559617324370	4.278315300303264	17.579096818430383
O	0.678320103917781	6.436847820741805	11.148700000000101
O	2.835959694741474	4.279218241284113	8.992779999999994
O	-1.479309475539881	4.279218241284144	13.304610000000086

O	0.678320103917781	6.436847820741805	15.460529999999977
O	2.835959694741474	4.279218241284113	13.304610000000086
O	-1.479309475539881	4.279218241284144	8.992779999999994
O	0.678320103917812	2.121578650460451	15.460529999999977
O	0.678320103917812	2.121578650460451	11.148700000000101
H	-1.957948069231834	2.644349068441185	22.203633037265138
H	-0.459707677359649	5.563366181603143	22.038428245199324
H	2.715779370175325	3.939891381558404	21.254731677967463
H	-3.717435982602871	4.306304568694157	21.232754395121908
O	-1.010719240632143	4.801132075768070	21.772787964098153
O	-1.393471407573590	2.109511407008672	21.612802706898524

0.50 ML H_2O coverage – 2/4 OH

40

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	-0.400855094987342	3.200763860731604	12.226650000000033
Cu	-0.400855094987342	1.042403451555298	10.070740000000047
Cu	-2.558494685811035	5.358403451555297	12.226650000000033
Cu	-0.400855094987373	7.516033031012959	16.538479999999911
Cu	-0.400855094987342	3.200763860731604	16.538479999999911
Cu	-0.400855094987342	1.042403451555298	14.382569999999925
Cu	1.756774484470320	3.200033031012960	10.070740000000047
Cu	-2.558494685811035	5.358403451555297	16.538479999999911
Cu	-0.400855094987373	5.357672621836652	14.382569999999925
Cu	1.756774484470320	3.200033031012960	14.382569999999925
Cu	-2.558494685811065	3.200033031012960	14.382569999999925
Cu	1.756774484470320	5.358403451555267	16.538479999999911

Cu	-0.400855094987373	7.516033031012959	12.226650000000033
Cu	-0.400855094987373	5.357672621836652	10.070740000000047
Cu	-2.558494685811065	3.200033031012960	10.070740000000047
Cu	1.756774484470320	5.358403451555267	12.226650000000033
Cu	-0.429118631649427	3.292385029797026	20.614893708002338
Cu	-0.410854474909554	1.038767026039777	18.612587264778004
Cu	-2.494182102359873	5.357935128090062	20.620918701119969
Cu	1.775176014693177	5.307805955016054	20.619272734376203
Cu	-0.480140759676174	7.560975332951791	20.614548534110376
Cu	-0.378620320791049	5.387549910402575	18.607171621840855
Cu	1.730009562721985	3.179706705727454	18.605290332280646
Cu	-2.555024600747266	3.210050891562235	18.609466584241936
O	-1.465669476487752	4.292771177385680	17.577230050924019
O	0.684048582342467	6.467534304147967	19.677092817252628
O	0.651773281351156	2.119845613737953	19.675690299826218
O	2.822796860430143	4.265696276920906	17.576803891488222
O	0.678320103917781	6.436847820741805	11.148700000000101
O	2.835959694741474	4.279218241284113	8.992779999999994
O	-1.479309475539881	4.279218241284144	13.304610000000086
O	0.678320103917781	6.436847820741805	15.460529999999977
O	2.835959694741474	4.279218241284113	13.304610000000086
O	-1.479309475539881	4.279218241284144	8.992779999999994
O	0.678320103917812	2.121578650460451	15.460529999999977
O	0.678320103917812	2.121578650460451	11.148700000000101
H	3.286990517192177	4.750916901612068	22.377373137556280
H	-0.906132077492770	4.873962764778827	22.329251478220339
O	-1.476201729717131	4.308000541297240	21.774253288287380

O 2.741001062791386 4.210407038999424 21.774821994001012

0.75 ML H_2O coverage – 0/4 OH

45

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu -2.189641687546193 4.172143809706766 13.529181908835975

Cu -0.064895365627976 6.202807662616213 13.447984958063564

Cu 0.093074574031842 8.153718352523001 15.091785767920459

Cu 2.288694973816049 2.460170807408186 15.105778579597555

Cu 2.253992873073093 4.424018037647317 13.579413887849562

Cu 0.116006879146529 2.225744638795727 13.664150710678898

Cu 0.501173973384105 4.248223931114332 15.398955088876010

Cu 1.786870593813765 6.500129234204579 15.130008124555308

Cu 2.157994995164452 6.473994995164452 11.467750000000004

Cu 0.000000000000000 0.000000000000000 11.467750000000004

Cu 0.000000000000000 4.316000000000000 7.155910000000008

Cu 0.000000000000000 4.316000000000000 11.467750000000004

Cu 2.157994995164453 2.157994995164453 7.155910000000008

Cu -2.158005004835517 4.316000000000000 5.000000000000021

Cu 0.000000000000000 2.157994995164483 5.000000000000021

Cu 0.000000000000000 0.000000000000000 7.155910000000008

Cu 0.000000000000000 6.473994995164483 9.311829999999899

Cu 2.157994995164483 4.316000000000000 5.000000000000021

Cu 2.157994995164452 6.473994995164452 7.155910000000008

Cu 2.157994995164483 4.316000000000000 9.311829999999899

Cu 0.000000000000000 6.473994995164483 5.000000000000021

Cu 2.157994995164453 2.157994995164453 11.467750000000004

Cu	-2.158005004835517	4.316000000000000	9.311829999999899
Cu	0.000000000000000	2.157994995164483	9.311829999999899
O	-1.082732489959445	5.392130561296833	10.393473064651655
O	-1.078881389756959	1.078982432330723	6.062799039881647
O	-1.073763247031772	1.084738052207774	10.405857780549217
O	-1.079015379241903	5.395085121055558	6.062137964689462
O	-3.236762126534094	3.237122467363394	8.248378516994340
O	1.078444846587071	3.236763838179582	8.248822905832320
O	-3.237899107197594	3.238202856211094	4.099662307190933
O	1.076719266382645	3.239469548156112	4.100636084093196
O	-1.105845749604121	5.145644943733195	14.635223977493560
O	1.141017594618261	3.298242894106127	12.524792285433678
O	-0.933557947886833	1.143689232057414	14.754355880643406
O	0.983906805644839	7.460714868853195	12.464782049150751
H	0.258093305538163	2.819418443554415	17.541478496656641
H	-2.845100635106845	3.303026304730442	17.011075236800902
H	-2.474583651115029	2.839957505641200	18.464428635423467
H	-0.575171278834202	0.991185873127916	16.914456683568979
H	0.457112093992220	0.574429982875723	18.018726950488141
H	-0.718676079215288	4.018787209330310	17.537152049550500
O	-2.521246649708201	3.641641447224067	17.903603087279912
O	0.232217561809656	3.810307332160767	17.338766016816340
O	-0.225452876708354	1.257957158979398	17.795404026667605

0.75 ML H_2O coverage – 1/4* OH

45

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	-2.079239692403527	4.218989524597304	13.560937206533030
Cu	0.046538592583228	6.314784299550253	13.538185574114348
Cu	0.066969330677832	8.348395609822278	15.485939710956520
Cu	2.208683179730727	2.234859353895372	15.253814861548618
Cu	2.255498719537453	4.307336567452451	13.474755357272024
Cu	0.078457105720380	2.102331472883138	13.513017365603853
Cu	0.362504683630211	3.972410211818529	15.493528637693709
Cu	2.104624014961747	6.291055710809712	15.487815654343455
Cu	2.157994995164452	6.473994995164452	11.467750000000004
Cu	0.000000000000000	0.000000000000000	11.467750000000004
Cu	0.000000000000000	4.316000000000000	7.155910000000008
Cu	0.000000000000000	4.316000000000000	11.467750000000004
Cu	2.157994995164453	2.157994995164453	7.155910000000008
Cu	-2.158005004835517	4.316000000000000	5.000000000000021
Cu	0.000000000000000	2.157994995164483	5.000000000000021
Cu	0.000000000000000	0.000000000000000	7.155910000000008
Cu	0.000000000000000	6.473994995164483	9.311829999999899
Cu	2.157994995164483	4.316000000000000	5.000000000000021
Cu	2.157994995164452	6.473994995164452	7.155910000000008
Cu	2.157994995164483	4.316000000000000	9.311829999999899
Cu	0.000000000000000	6.473994995164483	5.000000000000021
Cu	2.157994995164453	2.157994995164453	11.467750000000004
Cu	-2.158005004835517	4.316000000000000	9.311829999999899
Cu	0.000000000000000	2.157994995164483	9.311829999999899

O	-1.080384608785294	5.394996549635089	10.391248527942475
O	-1.078168302105032	1.078227512191886	6.053864922907340
O	-1.078098103747332	1.080886319898827	10.387861044160282
O	-1.078569593629782	5.394561773003780	6.054128770666892
O	-3.237067174743421	3.237020190725140	8.240743300942793
O	1.078890439001811	3.237116191843777	8.240342884399421
O	-3.235618838716405	3.235621090905225	4.100771406185639
O	1.080318273896836	3.235723373576881	4.098967031126739
O	-0.933267540449533	5.179375864282734	14.650216343418723
O	1.095465195434129	3.250006938097719	12.478134085345172
O	-0.935996403579592	0.984720227121710	14.575396306336080
O	1.057202654169236	7.526999684338826	12.525488049715324
H	-0.329201975067575	3.192834169872581	17.938230102854238
H	0.464422909487031	6.680854198229763	17.172083044406996
H	-0.146032935531137	1.005212136967942	19.121816919300741
H	0.547510380186410	0.962013258979965	17.733884396304969
H	-1.658814360255512	3.763733002150582	17.364013966713486
H	1.527869484351804	3.214411624955596	16.248915984402430
O	1.056289605704971	7.299968822396840	16.697946699044220
O	-0.711743911076010	4.001699321167498	17.509932493935494
O	0.305881298556567	1.566301133155596	18.466657599485998

0.75 ML H_2O coverage – 1/4 OH

44

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	-2.151289661803341	4.267578856883919	13.581093643721228
Cu	-0.008878318629508	6.330049099926699	13.563334357657595

Cu	-0.151706254172994	8.350279434915954	15.405372727640199
Cu	2.143197560879683	2.433727514060377	15.078048696493587
Cu	2.161279242875614	4.427749105551857	13.564183197068619
Cu	0.092381860260067	2.257111029204488	13.584946763677932
Cu	0.427652102092531	4.097064164118477	15.366453663958595
Cu	1.930213539376953	6.393773623112392	15.476902339528925
Cu	2.157994995164452	6.473994995164452	11.467750000000004
Cu	0.000000000000000	0.000000000000000	11.467750000000004
Cu	0.000000000000000	4.316000000000000	7.155910000000008
Cu	0.000000000000000	4.316000000000000	11.467750000000004
Cu	2.157994995164453	2.157994995164453	7.155910000000008
Cu	-2.158005004835517	4.316000000000000	5.000000000000021
Cu	0.000000000000000	2.157994995164483	5.000000000000021
Cu	0.000000000000000	0.000000000000000	7.155910000000008
Cu	0.000000000000000	6.473994995164483	9.311829999999899
Cu	2.157994995164483	4.316000000000000	5.000000000000021
Cu	2.157994995164452	6.473994995164452	7.155910000000008
Cu	2.157994995164483	4.316000000000000	9.311829999999899
Cu	0.000000000000000	6.473994995164483	5.000000000000021
Cu	2.157994995164453	2.157994995164453	11.467750000000004
Cu	-2.158005004835517	4.316000000000000	9.311829999999899
Cu	0.000000000000000	2.157994995164483	9.311829999999899
O	-1.082896553028049	5.391260755160719	10.400879428740534
O	-1.079100481651984	1.078951734770639	6.063698382432053
O	-1.077135856098427	1.080275701384380	10.401924717737591
O	-1.079136268463156	5.395089899221741	6.063993623273554
O	-3.237415461354617	3.236682693024320	8.250146776262124

O	1.079164543326386	3.237078835872065	8.249316142574857
O	-3.237653363975790	3.238525324377530	4.098696256442143
O	1.077093313764099	3.237083471318835	4.097453771195810
O	-1.051422082549786	5.248475671733740	14.704577148243821
O	1.142309511202966	3.303351978798107	12.464353760806206
O	-1.007609348651507	1.181946801208533	14.590518763644061
O	1.040059020089298	7.515486010305870	12.541285669525212
H	0.023911630401896	2.712058789592259	17.590930412755874
H	0.321568059124434	6.753526985259066	17.176098233039372
H	0.107487490795708	0.919404709240070	19.015414862932911
H	-3.608162224917612	4.672294872063944	17.684772147293756
H	-1.263196849778791	3.570296031596405	17.254489446450727
O	0.893610250154878	7.407351624276290	16.725161067174110
O	-0.282616345205289	3.618011499165044	17.292873913745776
O	0.584669668235881	1.189838323067040	18.211160745212567

0.75 ML H_2O coverage – 2/4 OH

43

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	-2.213631743772103	4.260262824867370	13.567496995356370
Cu	-0.046889995394904	6.407957689723795	13.555095399070975
Cu	-0.115552233161952	8.490769908245529	15.506112874363330
Cu	2.145613940604385	2.223888374033625	15.504381241661925
Cu	2.143099848521202	4.343478279514386	13.546556796513984
Cu	-0.015962764235047	2.163554472725504	13.552761195898972
Cu	0.001626462701262	4.198528853786009	15.596139263009860
Cu	2.011411000548069	6.512727485490105	15.584645456117649

Cu	2.157994995164452	6.473994995164452	11.467750000000004
Cu	0.000000000000000	0.000000000000000	11.467750000000004
Cu	0.000000000000000	4.316000000000000	7.155910000000008
Cu	0.000000000000000	4.316000000000000	11.467750000000004
Cu	2.157994995164453	2.157994995164453	7.155910000000008
Cu	-2.158005004835517	4.316000000000000	5.000000000000021
Cu	0.000000000000000	2.157994995164483	5.000000000000021
Cu	0.000000000000000	0.000000000000000	7.155910000000008
Cu	0.000000000000000	6.473994995164483	9.311829999999899
Cu	2.157994995164483	4.316000000000000	5.000000000000021
Cu	2.157994995164452	6.473994995164452	7.155910000000008
Cu	2.157994995164483	4.316000000000000	9.311829999999899
Cu	0.000000000000000	6.473994995164483	5.000000000000021
Cu	2.157994995164453	2.157994995164453	11.467750000000004
Cu	-2.158005004835517	4.316000000000000	9.311829999999899
Cu	0.000000000000000	2.157994995164483	9.311829999999899
O	-1.079162591568323	5.395204002380105	10.391039901212247
O	-1.078799053803761	1.078932212783062	6.053341294591880
O	-1.076086906010540	1.081365715637449	10.389711807952285
O	-1.078730529490824	5.394943274233189	6.053709048677495
O	-3.236935542150920	3.237127231776820	8.240755690041260
O	1.078964324487867	3.237094081772772	8.240708517741675
O	-3.235541426031602	3.235421358639266	4.099697449331852
O	1.080653909120867	3.235672936378857	4.099639247249605
O	-1.110185238706563	5.309252312005091	14.614845833237064
O	1.079705498398739	3.234910839907006	12.508051880326860
O	-1.131583435665499	1.131645818190058	14.612659649647645

O	1.028692132682576	7.505822916985932	12.508649592096221
H	0.817154575854743	2.641250459882154	17.342730919750348
H	0.272175574367953	6.813787963190024	17.158431669763377
H	0.016853229605540	1.013016525126177	19.012856049484032
H	-3.450953121982940	4.617410591963290	17.906124547258315
O	0.877310201024025	7.468515265429952	16.754563654591394
O	1.181763961549831	3.286330359110539	16.680870548737904
O	0.760851908248628	1.153452394839167	18.402423550056998

0.75 ML H_2O coverage – 3/4 OH

42

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	-0.400855094987342	3.200763860731604	12.226650000000033
Cu	-0.400855094987342	1.042403451555298	10.070740000000047
Cu	-2.558494685811035	5.358403451555297	12.226650000000033
Cu	-0.400855094987373	7.516033031012959	16.538479999999911
Cu	-0.400855094987342	3.200763860731604	16.538479999999911
Cu	-0.400855094987342	1.042403451555298	14.382569999999925
Cu	1.756774484470320	3.200033031012960	10.070740000000047
Cu	-2.558494685811035	5.358403451555297	16.538479999999911
Cu	-0.400855094987373	5.357672621836652	14.382569999999925
Cu	1.756774484470320	3.200033031012960	14.382569999999925
Cu	-2.558494685811065	3.200033031012960	14.382569999999925
Cu	1.756774484470320	5.358403451555267	16.538479999999911
Cu	-0.400855094987373	7.516033031012959	12.226650000000033
Cu	-0.400855094987373	5.357672621836652	10.070740000000047
Cu	-2.558494685811065	3.200033031012960	10.070740000000047

Cu	1.756774484470320	5.358403451555267	12.226650000000033
Cu	-0.202836433741180	3.255044193287089	20.840489230478124
Cu	-0.349357760540791	1.077308505891908	18.587353977027245
Cu	-2.468183521588819	5.520566650129926	20.851850190735831
Cu	1.869645009038633	5.331975095814419	20.626258190805469
Cu	-0.381658363998735	7.584418692465806	20.629413968889011
Cu	-0.428599938618712	5.314190702886059	18.681342611813935
Cu	1.785312608786431	3.211687786769732	18.568647181783696
Cu	-2.575101045280852	3.167982804442517	18.629989241331160
O	-1.495807838370516	4.263007784749015	17.597376751586783
O	0.679602408840923	6.396095412953130	19.688287959398281
O	0.736877146508695	2.140981307946064	19.626834116135093
O	2.867908601587096	4.311831189432072	17.563041083625965
O	0.678320103917781	6.436847820741805	11.148700000000101
O	2.835959694741474	4.279218241284113	8.992779999999994
O	-1.479309475539881	4.279218241284144	13.304610000000086
O	0.678320103917781	6.436847820741805	15.460529999999977
O	2.835959694741474	4.279218241284113	13.304610000000086
O	-1.479309475539881	4.279218241284144	8.992779999999994
O	0.678320103917812	2.121578650460451	15.460529999999977
O	0.678320103917812	2.121578650460451	11.148700000000101
H	-0.637692722448016	0.759693241551997	22.089121072951119
H	-0.741195495847255	4.974648905998587	22.462629682831782
H	0.871997083664093	2.255292979871564	23.046786884426506
O	-1.278040882975000	4.439833405705449	21.843306493291223
O	3.001179770297242	4.401317383728569	21.745530756304980
O	0.533240596444995	1.915447158226488	22.195107601485965

1.00 ML H_2O coverage – 0/4 OH

48

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	2.157994993440015	6.473994993440014	11.467750096282828
Cu	0.000000000000000	0.000000000000000	11.467750096282828
Cu	0.000000000000000	4.316000000000000	7.155909920364136
Cu	0.000000000000000	4.316000000000000	11.467750096282828
Cu	2.157994993440015	2.157994993440015	7.155909920364136
Cu	-2.158005006559985	4.316000000000000	5.000000094560074
Cu	0.000000000000000	2.157994993440015	5.000000094560074
Cu	0.000000000000000	0.000000000000000	7.155909920364136
Cu	0.000000000000000	6.473994993440015	9.311830008323588
Cu	2.157994993440015	4.316000000000000	5.000000094560074
Cu	2.157994993440015	6.473994993440014	7.155909920364136
Cu	2.157994993440015	4.316000000000000	9.311830008323588
Cu	0.000000000000000	6.473994993440015	5.000000094560074
Cu	2.157994993440015	2.157994993440015	11.467750096282828
Cu	-2.158005006559985	4.316000000000000	9.311830008323588
Cu	0.000000000000000	2.157994993440015	9.311830008323588
Cu	2.211972099702995	2.580385634877813	15.387220640340521
Cu	2.295029541441627	4.380671376882545	13.654604508420650
Cu	0.159298232335978	2.284934735328282	13.734745808167521
Cu	0.384808161417159	4.457256037169808	15.345963119725786
Cu	1.831830958990809	6.509538065387753	15.044003626563535
Cu	-2.225030593404242	4.236545879013955	13.479303718946108
Cu	-0.169890453605043	6.298520136188099	13.428479569048013

Cu	0.161324859056950	8.140167607906893	15.086531445372541
O	-1.250676170456420	5.296623428830864	14.588098716967870
O	1.161326987605771	3.319420379343317	12.542170568383460
O	-0.857227753398030	1.152606140356081	14.820366647160647
O	0.984558360639707	7.456343474271520	12.454614142649268
O	-1.079002503279992	5.395002503279992	10.389790052303100
O	-1.079002503279993	1.079002503279993	6.077960138539800
O	-1.079002503279993	1.079002503279993	10.389790052303100
O	-1.079002503279992	5.395002503279992	6.077960138539800
O	-3.236997496720007	3.236997496720007	8.233869964343864
O	1.079002503279993	3.236997496720007	8.233869964343864
O	-3.236997496720007	3.236997496720007	3.922040050580346
O	1.079002503279993	3.236997496720007	3.922040050580346
H	3.854033190246074	4.470906579279049	17.928341263942901
H	-1.035677021334063	3.895606611259380	17.616861135142777
H	-2.872376042698828	2.986203795399521	17.076740622518894
H	-1.930678441637574	2.200858833800461	18.054004563216459
H	-0.641540708904870	1.054242768592242	16.648322485007004
H	1.236077957313510	1.745443846084838	17.642420840501394
H	-1.489334887340329	5.960158528054444	17.641640205021240
H	0.494321089896726	4.164446236530317	18.002437048061566
O	-0.459636330594695	1.088630643628484	17.634915151359358
O	-0.223751609534613	4.482722582918381	17.421234340963203
O	2.072567136369614	2.266351613018159	17.483995632002205
O	-2.399994632942573	3.069122695732017	17.958704976118486

1.00 ML H_2O coverage – 1/4* OH

48

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	2.157994995164452	6.473994995164452	11.467750000000004
Cu	0.000000000000000	0.000000000000000	11.467750000000004
Cu	0.000000000000000	4.316000000000000	7.155910000000008
Cu	0.000000000000000	4.316000000000000	11.467750000000004
Cu	2.157994995164453	2.157994995164453	7.155910000000008
Cu	-2.158005004835517	4.316000000000000	5.000000000000021
Cu	0.000000000000000	2.157994995164483	5.000000000000021
Cu	0.000000000000000	0.000000000000000	7.155910000000008
Cu	0.000000000000000	6.473994995164483	9.311829999999899
Cu	2.157994995164483	4.316000000000000	5.000000000000021
Cu	2.157994995164452	6.473994995164452	7.155910000000008
Cu	2.157994995164483	4.316000000000000	9.311829999999899
Cu	0.000000000000000	6.473994995164483	5.000000000000021
Cu	2.157994995164453	2.157994995164453	11.467750000000004
Cu	-2.158005004835517	4.316000000000000	9.311829999999899
Cu	0.000000000000000	2.157994995164483	9.311829999999899
Cu	-1.625611350025240	6.528318157251682	15.991923129556572
Cu	2.100229659183888	4.396500396846964	13.606998932629903
Cu	-0.094106177741723	2.220539118491701	13.591502573954047
Cu	-0.210382990164926	4.482630259151133	15.716359111704822
Cu	-2.355625505285674	2.541196540917036	15.437765600891440
Cu	-2.144721594545950	4.454941227110883	13.459270176770719
Cu	0.014190820648821	6.573050161689473	13.464710116441507
Cu	-4.167325478538803	4.288642577764927	15.262747971342272

O	-1.079002502417759	5.395002502417759	10.389789999999952
O	-1.079002502417759	1.079002502417759	6.077960000000074
O	-1.079002502417759	1.079002502417759	10.389789999999952
O	-1.079002502417759	5.395002502417759	6.077960000000074
O	-3.236997497582241	3.236997497582241	8.233870000000060
O	1.079002502417759	3.236997497582241	8.233870000000060
O	-3.236997497582241	3.236997497582241	3.922039999999968
O	1.079002502417759	3.236997497582241	3.922039999999968
O	-1.111286129460235	5.567866766751411	14.487630729470125
O	1.075874158412101	3.241905065185883	12.553317606245775
O	-1.197165646603399	1.197051517607046	14.694058615632343
O	-3.174934508389260	3.299376138680421	12.461519332105283
H	3.570624211669784	3.719614116616835	18.288494803062495
H	-0.566819316415684	3.283466123897656	17.749238881746756
H	1.888469319836708	6.565338814709575	18.612997275216500
H	-1.131501265223498	1.351176855578234	18.262745837502866
H	-3.781850686848474	4.418978694471095	17.740513213640476
H	-1.983455407707571	6.296259774185122	18.313667769443754
H	1.081309806995426	3.432035854459509	17.628438421198116
H	-3.107315537336469	3.673439982411261	16.231030221905012
O	-0.063281822288279	0.121421151958451	18.520919345888917
O	0.167755653990852	3.909295649764422	17.452949461241115
O	2.384032941371983	2.766486524025443	17.738527101541205
O	-1.705618409999705	2.135604234553585	17.968558166745019

1.00 ML H_2O coverage – 1/4 OH

47

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	2.157994993440015	6.473994993440014	11.467750096282828
Cu	0.000000000000000	0.000000000000000	11.467750096282828
Cu	0.000000000000000	4.316000000000000	7.155909920364136
Cu	0.000000000000000	4.316000000000000	11.467750096282828
Cu	2.157994993440015	2.157994993440015	7.155909920364136
Cu	-2.158005006559985	4.316000000000000	5.000000094560074
Cu	0.000000000000000	2.157994993440015	5.000000094560074
Cu	0.000000000000000	0.000000000000000	7.155909920364136
Cu	0.000000000000000	6.473994993440015	9.311830008323588
Cu	2.157994993440015	4.316000000000000	5.000000094560074
Cu	2.157994993440015	6.473994993440014	7.155909920364136
Cu	2.157994993440015	4.316000000000000	9.311830008323588
Cu	0.000000000000000	6.473994993440015	5.000000094560074
Cu	2.157994993440015	2.157994993440015	11.467750096282828
Cu	-2.158005006559985	4.316000000000000	9.311830008323588
Cu	0.000000000000000	2.157994993440015	9.311830008323588
Cu	-1.234407785634537	6.522758071967353	16.023644629188411
Cu	2.016838669527019	4.484813272358950	13.589321908993226
Cu	-0.150900972902251	2.285429097265501	13.585728230526167
Cu	0.097119858917192	4.391310712497102	15.399431391430756
Cu	1.486868764223769	6.744960957113202	15.415653724681361
Cu	-2.362568902679540	4.253533538675909	13.597036961888055
Cu	-0.141618542404538	6.434249167058996	13.504536712880542
Cu	4.188750700874145	4.178881479616210	14.980321065382226

O	-1.296268698648212	5.396937867614618	14.525637304305468
O	1.077573244722153	3.242007318696350	12.554586761230695
O	-1.314534132665364	1.334723628289114	14.682300623283750
O	0.998080440641068	7.471662844103617	12.451149736840380
O	-1.079002503279992	5.395002503279992	10.389790052303100
O	-1.079002503279993	1.079002503279993	6.077960138539800
O	-1.079002503279993	1.079002503279993	10.389790052303100
O	-1.079002503279992	5.395002503279992	6.077960138539800
O	-3.236997496720007	3.236997496720007	8.233869964343864
O	1.079002503279993	3.236997496720007	8.233869964343864
O	-3.236997496720007	3.236997496720007	3.922040050580346
O	1.079002503279993	3.236997496720007	3.922040050580346
H	3.449887780702523	4.156783764926482	18.007932787558065
H	-0.427063519211067	3.450687028858154	17.555369985110296
H	1.493768614859429	7.029048624363343	18.083322756780003
H	-1.540219493476635	1.795475143428021	17.695887805083824
H	0.163884645163811	0.742456668424722	17.221782085179491
H	-1.627740520146928	6.434801277491247	18.409850276256872
H	1.246032075708202	3.383588945016979	17.539098285803131
O	0.396562056900162	3.902087051457491	17.252402939676237
O	2.643527525355634	2.831045958556233	17.746947336399774
O	-2.102554238048526	2.619147469359964	17.432293316312673
O	-0.397867784866982	0.753350025515198	18.026840725867991

1.00 ML H_2O coverage – 2/4 OH

46

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	2.157629579457693	6.474360409176308	11.467750000000004
Cu	0.000000000000000	0.000000000000000	11.467750000000004
Cu	0.000000000000000	4.316730829718614	7.155910000000008
Cu	0.000000000000000	4.316730829718614	11.467750000000004
Cu	2.158360409176307	2.158360409176307	7.155910000000008
Cu	-2.158370420542338	4.316730829718646	5.000000000000021
Cu	0.000000000000000	2.158360409176307	5.000000000000021
Cu	0.000000000000000	0.000000000000000	7.155910000000008
Cu	0.000000000000000	6.475091238894922	9.311829999999899
Cu	2.158360409176307	4.316730829718614	5.000000000000021
Cu	2.157629579457693	6.474360409176308	7.155910000000008
Cu	2.158360409176307	4.316730829718614	9.311829999999899
Cu	0.000000000000000	6.475091238894922	5.000000000000021
Cu	2.158360409176307	2.158360409176307	11.467750000000004
Cu	-2.158370420542338	4.316730829718646	9.311829999999899
Cu	0.000000000000000	2.158360409176307	9.311829999999899
Cu	-1.480659171235398	6.525599535689386	16.015979832750997
Cu	2.157030119190797	4.317371022920976	13.548437878910418
Cu	-0.018695281421772	2.160187350768539	13.545962885787768
Cu	-0.316312308843378	4.259078755134269	15.824146808809488
Cu	-2.132931717149117	2.265927910634566	15.523678603095497
Cu	-2.172256115559039	4.354639872949575	13.538236507882205
Cu	0.019098795199634	6.476051000100025	13.542216561306775
Cu	-4.157304062309260	4.297039448605425	15.460931717192523

O	-1.081023395933219	5.416932867502153	14.578264342501159
O	1.075164739399014	3.234753808791431	12.521703254330777
O	3.239375771670598	5.382159204313602	14.591629460704214
O	-3.226510864314085	3.247320941756015	12.497865330579017
O	-1.079185210271154	1.079185210271154	10.389789999999952
O	-1.079185210271154	1.079185210271154	6.077960000000074
O	-1.079185210271184	5.395916039989799	6.077960000000074
O	-3.237545619447461	3.237545619447461	8.233870000000060
O	1.079185210271154	3.237545619447461	8.233870000000060
O	-3.237545619447461	3.237545619447461	3.922039999999968
O	1.079185210271154	3.237545619447461	3.922039999999968
O	-1.079185210271184	5.395916039989799	10.389789999999952
H	0.600834686882464	0.646428861156398	17.981139363273382
H	-1.543009004732186	6.760977783530246	18.393422445808127
H	3.423902155934335	4.612016541169624	18.112205393392941
H	-0.197109059468727	2.630564659282517	17.719901587265156
H	0.663863815764743	7.186575843658996	17.247196848873365
H	1.206087571185779	3.406155942376452	17.592757349987444
O	-3.036680433532702	3.403277684978058	16.699512743668130
O	0.183767486961386	3.528102600509660	17.466924737160170
O	2.677829578646491	3.083480922072763	17.661583674091780
O	-0.245828379821019	1.040041576298629	18.282575512082360

1.00 ML H_2O coverage – 3/4 OH

45

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	2.157264289176517	6.473264289176518	11.467750000000004

Cu	0.000000000000000	0.000000000000000	11.467750000000004
Cu	0.000000000000000	4.316000000000000	7.155910000000008
Cu	0.000000000000000	4.316000000000000	11.467750000000004
Cu	2.157994995164453	2.157994995164453	7.155910000000008
Cu	-2.158005004835517	4.316000000000000	5.000000000000021
Cu	0.000000000000000	2.157994995164483	5.000000000000021
Cu	0.000000000000000	0.000000000000000	7.155910000000008
Cu	0.000000000000000	6.473994995164483	9.311829999999899
Cu	2.157994995164483	4.316000000000000	5.000000000000021
Cu	2.157264289176517	6.473264289176518	7.155910000000008
Cu	2.157994995164483	4.316000000000000	9.311829999999899
Cu	0.000000000000000	6.473994995164483	5.000000000000021
Cu	2.157994995164453	2.157994995164453	11.467750000000004
Cu	-2.158005004835517	4.316000000000000	9.311829999999899
Cu	0.000000000000000	2.157994995164483	9.311829999999899
Cu	-1.998364570364400	4.308145837482188	13.567051937292163
Cu	0.150983682268437	6.500841515093182	13.561274009694412
Cu	-3.951389559319397	4.222367165351377	15.605315143014117
Cu	-2.227075355821321	6.271459506713494	15.493713529225099
Cu	2.223064859503833	4.149898308136102	13.525707715776075
Cu	0.062852625182462	1.943854080132584	13.483392729831611
Cu	0.238046985059063	5.157865319490636	16.071387513283113
Cu	-1.772258420927304	2.183271400990653	15.496791188443607
O	-1.079002502417759	5.395002502417759	10.389789999999952
O	-1.079002502417759	1.079002502417759	6.077960000000074
O	-1.079002502417759	1.079002502417759	10.389789999999952
O	-1.079002502417759	5.395002502417759	6.077960000000074

O	-3.236997497582241	3.236997497582241	8.233870000000060
O	1.079002502417759	3.236997497582241	8.233870000000060
O	-3.236997497582241	3.236997497582241	3.922039999999968
O	1.079002502417759	3.236997497582241	3.922039999999968
O	-0.867505766259780	5.372501809597274	14.593222371950345
O	1.027560887698518	3.186960020908677	12.506116507527393
O	3.376714170919778	5.126848603559433	14.559042525236551
O	-3.153266151514390	3.308190689132268	12.503542185415972
H	0.763418644339269	5.278109024648410	18.417483821781889
H	-2.725867390520672	3.257758397112990	17.367932847007644
H	2.903414292320962	4.822828806451535	17.661477140095421
H	-0.029334037515035	1.296748755498625	17.434030572747133
H	1.017445176345178	3.308656636056428	17.133353988490544
O	3.896184965305744	4.701266773930935	17.567750940484881
O	-2.398898209950520	3.596172873047123	16.512213135042696
O	1.260509868556658	5.040172163169524	17.613949013396788
O	0.707886438203980	2.615599143940441	16.492420240402161

1.00 ML H_2O coverage – 4/4 OH

44

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	2.157629579457693	6.474360409176308	11.467750000000004
Cu	0.000000000000000	0.000000000000000	11.467750000000004
Cu	0.000000000000000	4.316730829718614	7.155910000000008
Cu	0.000000000000000	4.316730829718614	11.467750000000004
Cu	2.158360409176307	2.158360409176307	7.155910000000008
Cu	-2.158370420542338	4.316730829718646	5.000000000000021

Cu	0.000000000000000	2.158360409176307	5.000000000000021
Cu	0.000000000000000	0.000000000000000	7.155910000000008
Cu	0.000000000000000	6.475091238894922	9.311829999999899
Cu	2.158360409176307	4.316730829718614	5.000000000000021
Cu	2.157629579457693	6.474360409176308	7.155910000000008
Cu	2.158360409176307	4.316730829718614	9.311829999999899
Cu	0.000000000000000	6.475091238894922	5.000000000000021
Cu	2.158360409176307	2.158360409176307	11.467750000000004
Cu	-2.158370420542338	4.316730829718646	9.311829999999899
Cu	0.000000000000000	2.158360409176307	9.311829999999899
Cu	-2.016046192938706	6.314531548820980	15.794889353325944
Cu	2.284304614161617	4.328350490212329	13.497969691994042
Cu	0.103877911032103	2.148241205104658	13.543504805700502
Cu	0.074111053201252	4.229286263017576	15.782936309088207
Cu	2.307823054859598	6.317645362841216	15.793824116579529
Cu	-2.033461147834739	4.328270764627939	13.499035559764891
Cu	0.101235992151935	6.462763652135482	13.546229134964674
Cu	0.082416059743551	8.546241961544043	15.775349177820686
O	-0.918647986813983	5.326946103856854	14.559497738256251
O	1.126385926829638	3.282959885468652	12.509001884711246
O	-0.918024315533415	1.014413748531731	14.555899569907455
O	-3.191054681465245	3.280525478659860	12.510440622765818
O	-1.079185210271154	1.079185210271154	10.389789999999952
O	-1.079185210271154	1.079185210271154	6.077960000000074
O	-1.079185210271184	5.395916039989799	6.077960000000074
O	-3.237545619447461	3.237545619447461	8.233870000000060
O	1.079185210271154	3.237545619447461	8.233870000000060

O	-3.237545619447461	3.237545619447461	3.922039999999968
O	1.079185210271154	3.237545619447461	3.922039999999968
O	-1.079185210271184	5.395916039989799	10.389789999999952
H	3.124080302688697	5.046270957607497	17.914737317160668
H	0.427402414609032	2.353510257703149	17.150458015565530
H	0.435576912201939	6.680812983538464	17.144874544178350
H	-1.163850544531294	5.066600616761022	17.929154006504543
O	-0.755346382302171	1.152236094761458	17.158988167120128
O	1.096979281645930	7.341567257359245	16.761270661292862
O	-0.739378980923071	5.480066205353814	17.158919226734152
O	1.081498882931157	3.018432443074389	16.767169932762936

10.2. Ridge-dimer c(2×2) structures - p(2×2) unit cell

The H_2O monolayer structure displayed in **Figure 10** of the main article and in **Figure S5**:

0.25 ML H_2O coverage – 0/4 OH

96

Lattice vectors: [8.632, 0.000, 0.000 ; 0.000, 8.632, 0.000 ; 0.000, 0.000, 34.528]

Cu	8.222845999999986	4.726166000000029	15.537699999999974
Cu	8.619315999999985	0.606606000000015	15.156549999999974
Cu	8.561145999999985	6.600456000000030	13.663529999999975
Cu	4.368320000000002	4.998946000000030	15.282239999999975
Cu	4.291850000000002	2.320526000000022	13.725479999999974
Cu	2.327660000000002	4.670106000000029	13.625359999999976
Cu	6.976999999999991	2.340356000000023	15.273659999999975
Cu	4.400000000000000	4.535566000000030	11.411899999999974

Cu	4.400000000000000	2.379666000000023	9.255899999999983
Cu	2.244100000000002	4.535566000000030	9.255899999999983
Cu	6.555899999999992	2.379666000000023	11.411899999999974
Cu	4.400000000000000	4.535566000000030	7.099999999999991
Cu	4.400000000000000	2.379666000000023	4.944100000000000
Cu	6.555899999999992	4.535566000000030	4.944100000000000
Cu	6.555899999999992	2.379666000000023	7.099999999999991
Cu	3.862630000000002	0.289146000000013	15.663989999999975
Cu	4.411420000000001	6.950166000000030	13.507469999999975
Cu	2.176940000000002	0.106516000000013	13.569409999999975
Cu	6.414099999999993	6.495836000000029	15.144209999999974
Cu	4.400000000000000	0.223666000000014	11.411899999999974
Cu	4.400000000000000	6.691466000000030	9.255899999999983
Cu	2.244100000000002	0.223666000000014	9.255899999999983
Cu	6.555899999999992	6.691466000000030	11.411899999999974
Cu	4.400000000000000	0.223666000000014	7.099999999999991
Cu	4.400000000000000	6.691466000000030	4.944100000000000
Cu	6.555899999999992	0.223666000000014	4.944100000000000
Cu	6.555899999999992	6.691466000000030	7.099999999999991
Cu	0.111550000000002	2.632566000000023	13.506289999999975
Cu	6.491809999999993	4.426076000000030	13.687929999999975
Cu	2.084710000000002	2.083776000000022	15.073779999999974
Cu	0.088100000000002	4.535566000000030	11.411899999999974
Cu	0.088100000000002	2.379666000000023	9.255899999999983
Cu	6.555899999999992	4.535566000000030	9.255899999999983
Cu	2.244100000000002	2.379666000000023	11.411899999999974
Cu	0.088100000000002	4.535566000000030	7.099999999999991

Cu	0.088100000000002	2.379666000000023	4.944100000000000
Cu	2.244100000000002	4.535566000000030	4.944100000000000
Cu	2.244100000000002	2.379666000000023	7.099999999999991
Cu	6.541499999999993	0.403926000000015	13.609489999999976
Cu	2.621180000000002	6.631986000000030	15.242639999999975
Cu	0.088100000000002	0.223666000000014	11.411899999999974
Cu	0.088100000000002	6.691466000000030	9.255899999999983
Cu	6.555899999999992	0.223666000000014	9.255899999999983
Cu	2.244100000000002	6.691466000000030	11.411899999999974
Cu	0.088100000000002	0.223666000000014	7.099999999999991
Cu	0.088100000000002	6.691466000000030	4.944100000000000
Cu	2.244100000000002	0.223666000000014	4.944100000000000
Cu	2.244100000000002	6.691466000000030	7.099999999999991
O	8.634225999999984	4.980686000000031	17.566760000000002
O	1.166100000000002	7.769466000000028	6.022099999999995
O	7.633899999999988	1.301666000000017	3.866100000000004
O	1.166100000000002	7.769466000000028	10.333899999999979
O	7.633899999999988	1.301666000000017	8.177999999999988
O	1.056720000000002	7.661026000000028	14.717829999999974
O	7.700279999999987	1.369736000000018	12.456749999999975
O	1.166100000000002	3.457566000000027	6.022099999999995
O	7.633899999999988	5.613466000000029	3.866100000000004
O	1.166100000000002	3.457566000000027	10.333899999999979
O	7.633899999999988	5.613466000000029	8.177999999999988
O	1.152260000000002	3.736306000000028	14.700749999999974
O	7.543249999999988	5.527096000000030	12.492959999999975
O	5.477899999999997	7.769466000000028	6.022099999999995

O	3.322000000000002	1.301666000000017	3.866100000000004
O	5.477899999999997	7.769466000000028	10.333899999999979
O	3.322000000000002	1.301666000000017	8.177999999999988
O	5.356949999999998	8.111746000000020	14.720909999999975
O	3.285470000000002	1.264576000000018	12.508829999999975
O	5.477899999999997	3.457566000000027	6.022099999999995
O	3.322000000000002	5.613466000000029	3.866100000000004
O	5.477899999999997	3.457566000000027	10.333899999999979
O	3.322000000000002	5.613466000000029	8.177999999999988
O	5.357569999999998	3.354666000000027	14.873259999999975
O	3.406400000000002	5.691256000000029	12.455579999999975
O	3.200730000000002	0.875386000000015	17.445409999999999
O	0.663500000000002	1.972456000000020	17.951950000000011
O	7.029989999999990	0.436376000000014	19.058290000000028
O	5.152129999999999	2.426026000000023	18.198300000000014
O	2.539200000000002	6.015346000000029	18.202920000000013
O	4.751510000000000	4.647396000000031	19.477520000000037
O	6.593199999999992	6.519026000000030	18.449390000000019
H	3.897010000000002	1.522246000000018	17.833750000000009
H	2.298940000000002	1.277826000000017	17.608150000000006
H	0.202670000000002	1.856556000000020	17.068759999999994
H	0.552340000000002	2.935566000000025	18.130600000000012
H	6.343669999999993	1.116436000000018	18.850170000000027
H	7.884619999999988	0.876356000000016	18.852490000000024
H	5.465609999999997	2.737226000000024	17.321089999999998
H	4.992849999999999	3.290136000000027	18.740470000000023
H	7.927579999999987	5.560396000000029	17.993370000000009

H	0.886950000000002	5.409556000000030	17.773570000000007
H	3.002930000000002	5.981736000000030	17.310540000000000
H	2.561430000000002	6.964716000000029	18.443490000000018
H	3.908460000000002	5.082276000000030	19.213470000000033
H	5.449899999999998	5.328976000000029	19.308770000000035
H	6.127049999999994	6.579156000000030	17.585550000000001
H	6.774989999999992	7.487106000000029	18.712980000000023

10.3. Double-layer structures

Structures displayed in **Figure 11** of the main article.

0/4 OH

60

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	2.155909999999987	6.467739999999987	11.467750000000004
Cu	0.000000000000000	0.000000000000000	11.467750000000004
Cu	0.000000000000000	4.311830000000000	7.155910000000008
Cu	0.000000000000000	4.311830000000000	11.467750000000004
Cu	2.155909999999986	2.155909999999986	7.155910000000008
Cu	-2.155919999999983	4.311829999999999	5.000000000000021
Cu	0.000000000000000	2.155910000000016	5.000000000000021
Cu	0.000000000000000	0.000000000000000	7.155910000000008
Cu	0.000000000000000	6.467740000000017	9.311829999999899
Cu	2.155910000000017	4.311830000000000	5.000000000000021
Cu	2.155909999999987	6.467739999999987	7.155910000000008
Cu	2.155910000000017	4.311830000000000	9.311829999999899

Cu	0.000000000000000	6.467740000000017	5.000000000000021
Cu	2.155909999999986	2.155909999999986	11.467750000000004
Cu	-2.155919999999983	4.311829999999999	9.311829999999899
Cu	0.000000000000000	2.155910000000016	9.311829999999899
Cu	2.218735958323856	2.630914972350666	15.263861125566867
Cu	2.294120961245939	4.447543541118026	13.585249014019189
Cu	0.146981252255599	2.298879387544086	13.682083983510555
Cu	0.423719039103691	4.452230065263110	15.327871818784693
Cu	1.815674100662854	6.529537150783890	15.115458499212494
Cu	-2.221540659333630	4.231752346671378	13.512729206323533
Cu	-0.150923310431628	6.302962831710444	13.477109043714171
Cu	0.127040140233376	8.194280040982605	15.106991750326308
O	-1.077959999999991	5.389789999999991	10.389789999999952
O	-1.077959999999992	1.077959999999992	6.077960000000074
O	-1.077959999999992	1.077959999999992	10.389789999999952
O	-1.077959999999991	5.389789999999991	6.077960000000074
O	-3.233870000000008	3.233870000000008	8.233870000000060
O	1.077959999999992	3.233870000000008	8.233870000000060
O	-3.233870000000008	3.233870000000008	3.922039999999968
O	1.077959999999992	3.233870000000008	3.922039999999968
O	-2.247739468851606	3.385451302200352	18.077361441297203
O	-1.230037979979033	5.267286864754183	14.644975270746558
O	1.173450272918693	3.332725565496480	12.520430008941295
O	0.151775645225022	4.129629814988979	17.554781019966196
O	-2.302639254540261	6.298114496096944	17.403016214473695
O	-0.887430718702665	1.195977167065011	14.748021911661770
O	0.990612452380965	7.455707580466044	12.467317962413674

O	-0.318968809707679	1.050110522856067	17.743816084174629
O	-0.027027612965104	4.667970312030472	20.294346731187890
O	2.096380926588723	6.424674628145805	20.427747499403523
O	3.877539384047731	4.309528291469784	20.208605722928887
O	-2.067298501097455	6.526649602598816	20.225053721452408
H	-0.375819334880926	0.472936363573040	18.558551118050897
H	-0.744259678434888	3.634106674614186	17.667575895932227
H	-2.740574936210694	2.930485190980409	17.352112543182265
H	-2.261011113243345	2.790794126070515	18.893597885218128
H	3.525594833710733	4.942202916516021	16.990780502212893
H	1.143835343852146	1.421694769587620	17.463556344912075
H	-1.557467399959775	5.671782863927542	17.301569687317468
H	0.867797245598828	3.456555351598401	17.558628433375556
H	-1.467942402460106	5.759556235119618	20.419159456539287
H	1.311380395765513	5.826333118133610	20.529504286387759
H	0.081921764042059	4.460877859047402	19.325188523375942
H	0.022339371265860	3.813141346103221	20.762000106645779
H	2.111196436763318	2.149979867335292	19.246411198900926
H	3.291224332028606	3.490578517294415	20.315727926086286
H	-3.867077215792857	4.093676953518977	20.571840562187568
H	-1.456739247222060	1.476391654201660	20.483387274151688

1/4* OH

60

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	2.155909999999987	6.467739999999987	11.467750000000004
Cu	0.000000000000000	0.000000000000000	11.467750000000004

Cu	0.000000000000000	4.311830000000000	7.155910000000008
Cu	0.000000000000000	4.311830000000000	11.467750000000004
Cu	2.155909999999986	2.155909999999986	7.155910000000008
Cu	-2.155919999999983	4.311829999999999	5.000000000000021
Cu	0.000000000000000	2.155910000000016	5.000000000000021
Cu	0.000000000000000	0.000000000000000	7.155910000000008
Cu	0.000000000000000	6.467740000000017	9.311829999999899
Cu	2.155910000000017	4.311830000000000	5.000000000000021
Cu	2.155909999999987	6.467739999999987	7.155910000000008
Cu	2.155910000000017	4.311830000000000	9.311829999999899
Cu	0.000000000000000	6.467740000000017	5.000000000000021
Cu	2.155909999999986	2.155909999999986	11.467750000000004
Cu	-2.155919999999983	4.311829999999999	9.311829999999899
Cu	0.000000000000000	2.155910000000016	9.311829999999899
Cu	-1.616047117306474	6.407586272810383	15.990905215642885
Cu	2.158943571919075	4.330953700045632	13.590900390499257
Cu	-0.029156471073829	2.152536879536607	13.596479843226033
Cu	-0.305885426189132	4.293673187673639	15.709147450573564
Cu	-2.292740393244932	2.424513997456736	15.300306981908751
Cu	-2.163978366689189	4.393209131263175	13.440838164555480
Cu	-0.000285726028478	6.475221588726833	13.454655254882457
Cu	-4.113074461968537	4.113112941226559	15.292870794187813
O	-1.077959999999991	5.389789999999991	10.389789999999952
O	-1.077959999999992	1.077959999999992	6.077960000000074
O	-1.077959999999992	1.077959999999992	10.389789999999952
O	-1.077959999999991	5.389789999999991	6.077960000000074
O	-3.233870000000008	3.233870000000008	8.233870000000060

O	1.077959999999992	3.233870000000008	8.233870000000060
O	-3.233870000000008	3.233870000000008	3.922039999999968
O	1.077959999999992	3.233870000000008	3.922039999999968
O	-1.773284342966722	2.143773627226382	18.599537073548635
O	-1.104601215810219	5.455127453353765	14.484697618326141
O	1.072754261857356	3.232777173041590	12.547891102459360
O	0.142395507717683	3.733813735717468	17.409710900576790
O	2.382355635350911	2.792694059584135	17.654837169522320
O	3.223401805407083	5.387850565894937	14.693859744359870
O	-3.217125588958727	3.249438181419755	12.461259951038825
O	4.139810986086763	4.384336695622073	18.523439656032629
O	-1.489790025070393	2.232891515418813	21.367254314497256
O	0.357073312444277	4.196445198144262	20.674758763317275
O	-1.591463885729851	5.886961483191624	19.889841551005123
O	-3.763646228345833	4.586567405681769	21.127504615235555
H	3.457406795633434	3.700882949605779	18.114740533583351
H	-0.585750273874601	3.241134683166258	17.872416606773406
H	1.665431815958691	6.187600397126923	18.255339384589252
H	-1.173613456406194	1.329804267592740	18.511916559792393
H	-3.714186652364211	4.428556131689763	17.924553070186448
H	-1.834339863510797	6.480269553625208	18.463465194586419
H	1.114894916238225	3.286282862423531	17.593914234251645
H	-3.125883226526982	3.355471923044497	16.254830449121116
H	-3.397662643071561	3.805963303262970	21.586374188420564
H	-0.216753250675942	3.499803941488580	21.097974004777395
H	-1.704004850732828	2.184477846613161	20.399034771154696
H	-0.867565697948477	1.477494565057422	21.511573712040420

H	-4.051046127715892	4.277452459000856	20.225020498434830
H	-2.357920533195929	5.542705244562169	20.410689408800291
H	-0.822477025723145	5.292969982160362	20.124595734477346
H	0.952075380732492	4.541612564588554	21.364295214340714

1/4 OH

59

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	2.155909999999987	6.467739999999987	11.467750000000004
Cu	0.000000000000000	0.000000000000000	11.467750000000004
Cu	0.000000000000000	4.311830000000000	7.155910000000008
Cu	0.000000000000000	4.311830000000000	11.467750000000004
Cu	2.155909999999986	2.155909999999986	7.155910000000008
Cu	-2.155919999999983	4.311829999999999	5.000000000000021
Cu	0.000000000000000	2.155910000000016	5.000000000000021
Cu	0.000000000000000	0.000000000000000	7.155910000000008
Cu	0.000000000000000	6.467740000000017	9.311829999999899
Cu	2.155910000000017	4.311830000000000	5.000000000000021
Cu	2.155909999999987	6.467739999999987	7.155910000000008
Cu	2.155910000000017	4.311830000000000	9.311829999999899
Cu	0.000000000000000	6.467740000000017	5.000000000000021
Cu	2.155909999999986	2.155909999999986	11.467750000000004
Cu	-2.155919999999983	4.311829999999999	9.311829999999899
Cu	0.000000000000000	2.155910000000016	9.311829999999899
Cu	0.055994403708068	8.369179376385313	14.962901604925088
Cu	-0.792392654116775	6.254377870720829	15.988922987549195
Cu	2.101251392746307	4.370451175634821	13.589754797962383

Cu	-0.080558855979534	2.119772469189362	13.572661778318206
Cu	0.042658574160988	3.879458034388421	15.607178911163784
Cu	1.759432212860917	6.731844144481816	15.400709860805485
Cu	-2.170323101851792	4.164723483271540	13.580786614998830
Cu	0.076425394305178	6.282113854802286	13.504778892632238
O	-1.077959999999991	5.389789999999991	10.389789999999952
O	-1.077959999999992	1.077959999999992	6.077960000000074
O	-1.077959999999992	1.077959999999992	10.389789999999952
O	-1.077959999999991	5.389789999999991	6.077960000000074
O	-3.233870000000008	3.233870000000008	8.233870000000060
O	1.077959999999992	3.233870000000008	8.233870000000060
O	-3.233870000000008	3.233870000000008	3.922039999999968
O	1.077959999999992	3.233870000000008	3.922039999999968
O	-2.507478346055757	2.684489874114733	17.633593590474273
O	-0.919638563394304	5.092029107701050	14.546003011998279
O	1.062122282368901	3.203200079940128	12.556559206824968
O	0.773996077225444	3.098890254216019	17.190173974742329
O	-1.022412232025641	7.118067358762103	17.626483815870870
O	3.117053571079277	5.468376858845199	14.725591810358130
O	1.030168896854844	7.500591182568916	12.456017903761200
O	-0.636913272748102	0.924225360022263	18.207834935407814
O	-1.695128823024167	3.057186061743554	20.456665879224762
O	0.461418264165182	4.338493381018063	19.578817454224957
O	-1.527040769169014	6.449564508535219	20.172349910395617
O	0.302878977212029	1.034025133023885	20.671512213039367
H	1.804694614678070	3.008822401975339	17.260714714482894
H	3.585558876239655	4.259965141543308	17.882230817322153

H	0.545980001476791	3.631372564872050	18.016781327390678
H	0.827370336523208	6.861639424963224	17.742024120049891
H	2.308884729901292	6.152018699230803	17.845961178612516
H	-0.018509405907095	1.437008456800513	17.634072947292765
H	-1.214944993645489	6.665777940815808	18.499080053332897
H	-3.904660445964123	4.475336438165397	21.099063482332291
H	-0.323384538594169	3.829408844423192	19.973222763919104
H	-2.066775755860495	2.874252932002340	19.560597191365069
H	-1.241674253102982	2.226421721066218	20.741479852641280
H	-0.004483630581519	0.856636162955382	19.724976868826552
H	-2.358415125329397	5.956817160895417	20.422767403626288
H	-0.779910294181745	5.838771950879737	20.343853298182630
H	1.253480727839200	3.998108882623846	20.041232569131729

2/4 OH

58

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	2.155179999999997	6.467009999999997	11.467750000000004
Cu	0.000000000000000	0.000000000000000	11.467750000000004
Cu	0.000000000000000	4.311830000000000	7.155910000000008
Cu	0.000000000000000	4.311830000000000	11.467750000000004
Cu	2.155909999999986	2.155909999999986	7.155910000000008
Cu	-2.155919999999983	4.311829999999999	5.000000000000021
Cu	0.000000000000000	2.155910000000016	5.000000000000021
Cu	0.000000000000000	0.000000000000000	7.155910000000008
Cu	0.000000000000000	6.467740000000017	9.311829999999899
Cu	2.155910000000017	4.311830000000000	5.000000000000021

Cu	2.155179999999997	6.467009999999997	7.155910000000008
Cu	2.155910000000017	4.311830000000000	9.311829999999899
Cu	0.000000000000000	6.467740000000017	5.000000000000021
Cu	2.155909999999986	2.155909999999986	11.467750000000004
Cu	-2.155919999999983	4.311829999999999	9.311829999999899
Cu	0.000000000000000	2.155910000000016	9.311829999999899
Cu	0.088383302271137	6.389423337183058	13.514778275220765
Cu	-3.973237393979474	4.147808231308995	15.455958032572063
Cu	-1.316078432515075	6.430979011265868	15.970145583078487
Cu	2.243929362009874	4.245111003487943	13.529018517161520
Cu	0.059947549165782	2.081636015404020	13.528844212558168
Cu	-0.176479101380902	4.124530182982667	15.813493826476865
Cu	-1.958351420334761	2.101458514219829	15.503342003037099
Cu	-2.080305373494257	4.286366378065924	13.511234039830958
O	-1.077959999999992	1.077959999999992	10.389789999999952
O	-1.077959999999992	1.077959999999992	6.077960000000074
O	-1.077959999999991	5.389789999999991	6.077960000000074
O	-3.233870000000008	3.233870000000008	8.233870000000060
O	1.077959999999992	3.233870000000008	8.233870000000060
O	-3.233870000000008	3.233870000000008	3.922039999999968
O	1.077959999999992	3.233870000000008	3.922039999999968
O	-1.077959999999991	5.389789999999991	10.389789999999952
O	-2.837309924055293	3.250944414549203	16.673198393875406
O	-0.940948658390785	5.276261785288268	14.566766695338293
O	1.080614705301119	3.235307013802361	12.518493816298729
O	0.357611135373033	3.371695171713458	17.438058996540576
O	2.829197738038669	3.022840660374879	17.593405531618661

O	-0.904668960518928	0.905936774206404	14.575807892886928
O	-3.219339153612692	3.244304516746109	12.495276096303497
O	-0.146812404575609	0.839360763138403	18.324505559412732
O	-2.400846029364752	3.561734729642883	20.246901633026525
O	-0.969232381039036	5.769954364167614	19.816407228122991
O	1.831909730244234	3.520140370556095	20.964914924144836
O	-0.852542678786065	1.476893084073476	20.873866708421872
H	0.884994033467463	7.030980547580084	17.246056538680214
H	1.398269645149426	3.263321678502916	17.554965732235534
H	-3.552638354820252	4.781219880994464	18.276563809964372
H	-1.314070212179267	6.701016294749403	18.341613342746225
H	3.580561293470247	4.366198402449580	18.015212182460154
H	-0.019691156656869	2.477695887844154	17.661954055362141
H	2.868597211024000	5.033258914656197	21.125026282816503
H	-1.445013360472478	4.888400515530378	19.951570679552034
H	-2.982778486365201	3.779994661848014	20.997488281196063
H	-1.831688835929922	2.773691346889464	20.540862269947837
H	-0.551869566413035	1.235692995097231	19.949631565634352
H	1.076266842687323	3.083977266546742	21.400840152346934
H	2.401151280815461	2.778779707911064	20.633354782102572
H	-0.017820325830129	5.582165604945029	19.918211087043009

3/4 OH

57

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	2.155179999999997	6.467009999999997	11.467750000000004
Cu	0.000000000000000	0.000000000000000	11.467750000000004

Cu	0.000000000000000	4.311830000000000	7.155910000000008
Cu	0.000000000000000	4.311830000000000	11.467750000000004
Cu	2.155909999999986	2.155909999999986	7.155910000000008
Cu	-2.155919999999983	4.311829999999999	5.000000000000021
Cu	0.000000000000000	2.155910000000016	5.000000000000021
Cu	0.000000000000000	0.000000000000000	7.155910000000008
Cu	0.000000000000000	6.467740000000017	9.311829999999899
Cu	2.155910000000017	4.311830000000000	5.000000000000021
Cu	2.155179999999997	6.467009999999997	7.155910000000008
Cu	2.155910000000017	4.311830000000000	9.311829999999899
Cu	0.000000000000000	6.467740000000017	5.000000000000021
Cu	2.155909999999986	2.155909999999986	11.467750000000004
Cu	-2.155919999999983	4.311829999999999	9.311829999999899
Cu	0.000000000000000	2.155910000000016	9.311829999999899
Cu	-0.018343577726309	2.142924445908445	13.473921250263823
Cu	0.123499226282163	5.135253346076018	16.209359055850872
Cu	-2.088556505805049	2.513685019411621	15.345559164703353
Cu	-2.043863234713439	4.439590352905785	13.539353759313526
Cu	0.062420723069117	6.552012750709645	13.575689176076660
Cu	0.165058858768241	0.270999633568270	15.505826393084094
Cu	2.014398035568600	2.309010956458772	15.418362388497519
Cu	2.172949542677290	4.330941093069410	13.480268841049316
O	-1.077959999999991	5.389789999999991	10.389789999999952
O	-1.077959999999992	1.077959999999992	6.077960000000074
O	-1.077959999999992	1.077959999999992	10.389789999999952
O	-1.077959999999991	5.389789999999991	6.077960000000074
O	-3.233870000000008	3.233870000000008	8.233870000000060

O	1.077959999999992	3.233870000000008	8.233870000000060
O	-3.233870000000008	3.233870000000008	3.922039999999968
O	1.077959999999992	3.233870000000008	3.922039999999968
O	-1.150852386965832	1.143759767715664	14.524528024166685
O	-3.156177813302274	3.315061141899515	12.513449415005571
O	-0.849045283638530	1.195901250959293	17.725480801190354
O	-2.810924152772905	3.772389746596565	16.498352072610700
O	-0.981916432796806	5.485621791215637	14.681099900034200
O	1.081828170586730	3.235820811851560	12.491937783213549
O	0.794391643384210	5.902531183275393	17.801089130226135
O	0.815377391659931	3.295305501345269	16.476729200585986
O	-2.450060427452466	3.105477711137083	20.138123934418626
O	-0.881645861478189	5.290207601493984	19.868151453922174
O	1.754436181033169	3.099927315836169	19.035038067307031
O	-0.221137903455139	1.490882361309676	20.252732931005493
H	0.261512658702637	5.523777595211280	18.548858837953240
H	1.058720273111440	7.493936743655128	17.174422908179938
H	2.455305509892757	5.598886900665457	17.759477130626319
H	-0.479283637205807	2.027419123362397	17.338909747116851
H	1.227077710204495	3.295762930610565	17.400527176925518
H	0.139544704494121	0.704786233791334	20.702296336312813
H	-1.476605248460756	4.480475631126509	19.943501208029225
H	1.494862944315653	7.057626580779088	19.296801592982902
H	-1.749773989549942	2.445154509851789	20.391293021708105
H	-0.426025015758452	1.207769384510400	19.301237308538603
H	1.031941632712124	2.683329472277728	19.568515393821123
H	-1.814226506992211	6.783364970463729	19.198656397434021

H -0.417398025881475 5.379804578472919 20.718283577127618

4/4 OH

56

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	2.155179999999997	6.467009999999997	11.467750000000004
Cu	0.000000000000000	0.000000000000000	11.467750000000004
Cu	0.000000000000000	4.311830000000000	7.155910000000008
Cu	0.000000000000000	4.311830000000000	11.467750000000004
Cu	2.155909999999986	2.155909999999986	7.155910000000008
Cu	-2.155919999999983	4.311829999999999	5.000000000000021
Cu	0.000000000000000	2.155910000000016	5.000000000000021
Cu	0.000000000000000	0.000000000000000	7.155910000000008
Cu	0.000000000000000	6.467740000000017	9.311829999999899
Cu	2.155910000000017	4.311830000000000	5.000000000000021
Cu	2.155179999999997	6.467009999999997	7.155910000000008
Cu	2.155910000000017	4.311830000000000	9.311829999999899
Cu	0.000000000000000	6.467740000000017	5.000000000000021
Cu	2.155909999999986	2.155909999999986	11.467750000000004
Cu	-2.155919999999983	4.311829999999999	9.311829999999899
Cu	0.000000000000000	2.155910000000016	9.311829999999899
Cu	2.381767094369526	6.229200494788958	15.832623171357925
Cu	-1.938777659972234	4.384798670103137	13.502162278500697
Cu	0.199178678154182	6.521421573042209	13.526467997330622
Cu	0.111599768988099	8.476608233684331	15.798512257485630
Cu	-1.795551233234719	6.412972146818327	15.797124186246151
Cu	2.212364228851943	4.217634269554598	13.536002825582118

Cu	0.036957973537286	2.040509435538541	13.518231316172319
Cu	0.268704324160847	4.338305827386897	15.779334781464998
O	-1.077959999999992	1.077959999999992	10.389789999999952
O	-1.077959999999992	1.077959999999992	6.077960000000074
O	-1.077959999999991	5.389789999999991	6.077960000000074
O	-3.233870000000008	3.233870000000008	8.233870000000060
O	1.077959999999992	3.233870000000008	8.233870000000060
O	-3.233870000000008	3.233870000000008	3.922039999999968
O	1.077959999999992	3.233870000000008	3.922039999999968
O	-1.077959999999991	5.389789999999991	10.389789999999952
O	-3.020231266940584	3.092674559204116	16.742980669172631
O	-0.782399972182324	5.370482670314010	14.542309150009352
O	1.054056639914750	3.207577407972589	12.515342375518765
O	-1.067580613635450	5.027992395046632	17.136985824259771
O	1.289555271797024	3.123548100286027	16.764009553743254
O	3.366551019909925	5.203272231686817	14.559083385423909
O	-3.109323241769974	3.356357691071989	12.503613975461107
O	-0.474249576120709	1.352384847877322	17.068019732729613
O	-0.809602030481004	5.592082242201490	19.613638705648235
O	1.257540456972150	7.257395676657344	19.312178196161110
O	-1.049859294246393	1.093809612754920	19.681151310270486
O	1.683234583876158	3.330879290531692	19.520558365302975
H	-0.694395209584890	1.184237204607164	18.029569332427876
H	0.554073015507805	2.389528103712233	16.973325343470147
H	1.212079402912958	7.307898800868350	17.774174731230715
H	-1.778575836054659	4.336351346995828	17.086114953777880
H	2.226814741464970	2.519093120311973	19.702761440406235

H	0.497680398422212	6.638822910221778	19.535438235458159
H	-0.888699817143658	5.308021233894563	18.620251876986018
H	-0.609255578086817	4.782366422561601	20.115026750223262
H	1.546375831244413	3.317488883153952	18.534159135052441
H	2.694925522324763	4.557198890980307	19.723331411435211
H	-0.214253508719371	0.922404816907274	20.150014553298142
H	-2.246279586896255	2.427727267155142	19.562692253238730

10.4. (3,0;1,1) structures

Structures for the (3,0;1,1) surface reconstruction as displayed in **Figure 12** of the main article and in **Figure S2** and **Figure S3**:

Single H_2O adsorption

57

Lattice vectors: [8.632, -4.316, 0.000 ; 4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	9.701619999999977	-1.077960000000004	3.233870000000039
Cu	7.545699999999977	-1.077959999999992	1.077960000000053
Cu	5.389790000000015	3.233870000000001	3.233870000000039
Cu	3.233870000000007	1.077959999999990	3.233870000000039
Cu	9.701619999999982	1.077960000000014	1.077960000000053
Cu	7.545699999999982	1.077960000000027	3.233870000000039
Cu	3.233870000000033	-1.077959999999997	1.077960000000053
Cu	5.389790000000009	1.077959999999978	1.077960000000053
Cu	5.389790000000033	-1.077960000000010	3.233870000000039
Cu	3.233870000000014	3.233870000000014	1.077960000000053

Cu	1.077960000000002	1.077960000000002	1.077960000000053
Cu	7.545700000000002	-3.233869999999984	3.233870000000039
Cu	9.701619999999977	-1.077960000000004	7.545730000000058
Cu	7.545699999999977	-1.077959999999992	5.389820000000072
Cu	5.389790000000015	3.233870000000001	7.545730000000058
Cu	3.233870000000007	1.077959999999990	7.545730000000058
Cu	9.701619999999982	1.077960000000014	5.389820000000072
Cu	7.545699999999982	1.077960000000027	7.545730000000058
Cu	3.233870000000033	-1.077959999999997	5.389820000000072
Cu	5.389790000000009	1.077959999999978	5.389820000000072
Cu	5.389790000000033	-1.077960000000010	7.545730000000058
Cu	3.233870000000014	3.233870000000014	5.389820000000072
Cu	1.077960000000002	1.077960000000002	5.389820000000072
Cu	7.545700000000002	-3.233869999999984	7.545730000000058
Cu	8.069773539237181	-3.936102652094050	11.549491301446603
Cu	7.279171866892868	-0.458072166453719	9.775449368243907
Cu	5.348379547132419	0.156931049686105	11.278122073938103
Cu	5.241378706361980	2.848551155476986	10.858441954837616
Cu	9.306734485720986	1.405895767134881	9.739408097264414
Cu	7.318893336488102	1.662987011751127	11.148156403549494
Cu	2.837946675832770	-1.014637966437880	9.383414735269843
Cu	5.630248714694977	1.276673287715230	9.164514029490185
Cu	6.622759547352117	-1.943243297851926	11.529059846650066
Cu	3.001532659489632	2.801210494346260	9.342867924433733
Cu	1.240344247820560	1.036629662561714	9.372800515854234
Cu	10.103203224668693	-1.753094528727107	11.326730889843031
O	6.467749999999970	-2.155919999999995	2.155909999999986

O	4.311830000000006	-0.000000000000025	0.000000000000000
O	8.623659999999980	0.000000000000012	0.000000000000000
O	2.155910000000011	2.155910000000011	2.155909999999986
O	6.467740000000015	2.155919999999981	2.155909999999986
O	4.311829999999986	4.311829999999986	0.000000000000000
O	6.467749999999970	-2.155919999999995	6.467779999999911
O	4.311830000000006	-0.000000000000025	4.311860000000019
O	8.623659999999980	0.000000000000012	4.311860000000019
O	2.155910000000011	2.155910000000011	6.467779999999911
O	6.467740000000015	2.155919999999981	6.467779999999911
O	4.311829999999986	4.311829999999986	4.311860000000019
O	8.402258829078173	-2.157811246205210	11.798486486794626
O	4.293306295326938	-0.018069240697099	8.574865049289958
O	8.717115944121229	0.060160526936982	8.571388095268309
O	3.308822539837382	2.909547083689697	11.387352008588300
O	4.810231324057388	-1.837535012066797	11.296422391067034
O	12.810534937054964	-0.094900110406162	8.563726091951777
O	3.945887676021140	0.662146076701248	12.694090285616150
H	3.237990755105018	-0.010418497288660	12.644931209703998
H	3.562645052216784	1.522659426783829	12.344325222133987

H_2O ML

72

Lattice vectors: [8.632, -4.316, 0.000 ; 4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	9.701619994703984	-1.077960007018801	3.233869869783788
Cu	7.545700037845587	-1.077960005272685	1.077960013796806
Cu	5.389789991189014	3.233870032584503	3.233869869783788

Cu	3.233869994750415	1.077959996473200	3.233869869783788
Cu	9.701620034330386	1.077959991212114	1.077960013796806
Cu	7.545699991235415	1.077960036076472	3.233869869783788
Cu	3.233869972371453	-1.077959984510274	1.077960013796806
Cu	5.389789951608811	1.077959994727084	1.077960013796806
Cu	5.389790041337557	-1.077960003503500	3.233869869783788
Cu	3.233869991212014	3.233869991212014	1.077960013796806
Cu	1.077959998242415	1.077959998242415	1.077960013796806
Cu	7.545700028448421	-3.233870012947065	3.233869869783788
Cu	9.701619994703984	-1.077960007018801	7.545729966357012
Cu	7.545700037845587	-1.077960005272685	5.389820140553167
Cu	5.389789991189014	3.233870032584503	7.545729966357012
Cu	3.233869994750415	1.077959996473200	7.545729966357012
Cu	9.701620034330386	1.077959991212114	5.389820140553167
Cu	7.545699991235415	1.077960036076472	7.545729966357012
Cu	3.233869972371453	-1.077959984510274	5.389820140553167
Cu	5.389789951608811	1.077959994727084	5.389820140553167
Cu	5.389790041337557	-1.077960003503500	7.545729966357012
Cu	3.233869991212014	3.233869991212014	5.389820140553167
Cu	1.077959998242415	1.077959998242415	5.389820140553167
Cu	7.545700028448421	-3.233870012947065	7.545729966357012
Cu	8.327495329698628	-3.892596844431143	11.379236961042102
Cu	7.207581801564060	-0.917400097593664	9.364582593469772
Cu	5.513623966539337	0.072721255570753	11.098089945555691
Cu	5.276939884215540	2.515758925939260	10.998678415851167
Cu	9.327438922601818	1.475243991333564	9.687167367570600
Cu	7.435180570654982	1.580966305571556	11.414319167246843

Cu	2.852545452993586	-1.249896267872957	9.458890235871008
Cu	5.583552552773845	1.217357464541581	9.058413594105334
Cu	6.744938630525381	-2.012941166546491	11.468640588474681
Cu	3.106731918277973	2.821458642709537	9.283317201538171
Cu	1.317053241812393	1.122990579159260	9.280887538820043
Cu	10.275181304300313	-1.758583345841263	11.255521698550581
O	6.467749999953568	-2.155920003492000	2.155910006900938
O	4.311829953366426	-0.000000003515300	0.000000000000000
O	8.623660036087973	-0.000000007030300	0.000000000000000
O	2.155909992969599	2.155909992969599	2.155910006900938
O	6.467739989500829	2.155919992946400	2.155910006900938
O	4.311829989454399	4.311829989454399	0.000000000000000
O	6.467749999953568	-2.155920003492000	6.467779882704766
O	4.311829953366426	-0.000000003515300	4.311860096573439
O	8.623660036087973	-0.000000007030300	4.311860096573439
O	2.155909992969599	2.155909992969599	6.467779882704766
O	6.467739989500829	2.155919992946400	6.467779882704766
O	4.311829989454399	4.311829989454399	4.311860096573439
O	8.566184698847657	-2.109387988453376	11.776265361176609
O	4.201690689534574	-0.105712451399148	8.578332017127535
O	8.709340792511325	0.070008726293146	8.594510204625054
O	3.450449845378492	2.968289193917159	11.353217430478759
O	4.931276364356452	-1.748538343616651	11.232959644298253
O	4.255582696192900	4.272744899008716	8.567859317399712
O	3.354288237748939	3.112842003157829	14.089314587506770
O	8.225239798510206	-1.396693537771234	14.288787933400393
O	6.049705000104472	3.420844084226559	13.957491748360974

O	10.512761910784409	1.202046515827917	13.816472533791023
O	7.869389379151413	1.211126325820435	13.437732990990733
O	1.767796312903587	1.337909959552401	15.358109519000404
H	3.309246821826450	2.875844163360210	13.121951389027647
H	2.843022421127055	2.414043778452340	14.589560401811248
H	8.483230720087329	-1.688164002283983	13.352354869937805
H	8.909456160376742	-1.807371522311887	14.868756247166907
H	5.110156148169725	3.121785032577400	14.104861643636148
H	6.646487854313056	2.635329859351231	13.963589886301170
H	6.843903060735845	-2.446938757982268	14.192775224136694
H	10.946185293732867	0.320647494441784	13.968618937352172
H	8.860375838098117	1.368343476245878	13.551163745296060
H	7.788709415412315	0.296304923177592	13.823291035428531
H	1.816150970711246	0.444708690640498	14.874734648329655
H	1.927574606567346	1.151855060084857	16.298818365869597

1:5 OH:H_2O ML

71

Lattice vectors: [8.632, -4.316, 0.000 ; 4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	9.701619994703984	-1.077960007018801	3.233869869783788
Cu	7.545700037845587	-1.077960005272685	1.077960013796806
Cu	5.389789991189014	3.233870032584503	3.233869869783788
Cu	3.233869994750415	1.077959996473200	3.233869869783788
Cu	9.701620034330386	1.077959991212114	1.077960013796806
Cu	7.545699991235415	1.077960036076472	3.233869869783788
Cu	3.233869972371453	-1.077959984510274	1.077960013796806
Cu	5.389789951608811	1.077959994727084	1.077960013796806

Cu	5.389790041337557	-1.077960003503500	3.233869869783788
Cu	3.233869991212014	3.233869991212014	1.077960013796806
Cu	1.077959998242415	1.077959998242415	1.077960013796806
Cu	7.545700028448421	-3.233870012947065	3.233869869783788
Cu	9.701619994703984	-1.077960007018801	7.545729966357012
Cu	7.545700037845587	-1.077960005272685	5.389820140553167
Cu	5.389789991189014	3.233870032584503	7.545729966357012
Cu	3.233869994750415	1.077959996473200	7.545729966357012
Cu	9.701620034330386	1.077959991212114	5.389820140553167
Cu	7.545699991235415	1.077960036076472	7.545729966357012
Cu	3.233869972371453	-1.077959984510274	5.389820140553167
Cu	5.389789951608811	1.077959994727084	5.389820140553167
Cu	5.389790041337557	-1.077960003503500	7.545729966357012
Cu	3.233869991212014	3.233869991212014	5.389820140553167
Cu	1.077959998242415	1.077959998242415	5.389820140553167
Cu	7.545700028448421	-3.233870012947065	7.545729966357012
Cu	7.762869205163559	-3.421346152897526	10.995565161954039
Cu	7.306016921122989	-0.494642166390922	9.863751401835382
Cu	5.718032862361789	-0.179784184691444	11.783146948243770
Cu	5.273648718148056	3.235987366314216	10.953989059002911
Cu	9.330492663481852	1.447142642386816	9.665761567689550
Cu	7.248069410403986	1.769657786176536	11.172162810906416
Cu	2.897872199042693	-1.026343462787857	9.357962108102948
Cu	5.553414678237105	1.329744084908751	9.425055001419123
Cu	5.464054129780339	-2.667705907259777	12.406223227127363
Cu	3.213186278015521	2.744792371386670	9.288804090831240
Cu	1.334147695921891	1.107122952234071	9.359527064340517

Cu	9.978764838757456	-1.315825719059414	10.965234557833993
O	6.467749999953568	-2.155920003492000	2.155910006900938
O	4.311829953366426	-0.000000003515300	0.000000000000000
O	8.623660036087973	-0.000000007030300	0.000000000000000
O	2.155909992969599	2.155909992969599	2.155910006900938
O	6.467739989500829	2.155919992946400	2.155910006900938
O	4.311829989454399	4.311829989454399	0.000000000000000
O	6.467749999953568	-2.155920003492000	6.467779882704766
O	4.311829953366426	-0.000000003515300	4.311860096573439
O	8.623660036087973	-0.000000007030300	4.311860096573439
O	2.155909992969599	2.155909992969599	6.467779882704766
O	6.467739989500829	2.155919992946400	6.467779882704766
O	4.311829989454399	4.311829989454399	4.311860096573439
O	8.201267132237207	-1.656027235071581	11.187465074964756
O	4.342497588203540	0.049437020570763	8.578282902028196
O	8.716349270928395	0.072073835351453	8.552093039432380
O	11.784736567766252	-0.946165068337563	11.181937780758140
O	4.800110279929966	-1.611527597946025	11.047276451834142
O	12.894686406871806	-0.004170763304757	8.550154940056427
O	11.732290564523840	-1.182863574132331	13.789352718156922
O	8.116059969080531	-1.422402709301759	13.873926485404263
O	5.650881799237547	3.370919329957770	13.213996575077001
O	10.466568450446509	1.121585018466334	14.084513740560801
O	6.655217998884684	0.980065023828717	12.945204460107451
O	1.629162606910169	1.158080521072705	14.762692627933323
H	11.637099954154825	-1.233564994464179	12.779234828634774
H	2.662789549195098	2.326710135846446	14.188487916807658

H	8.195833991040814	-1.516562884301785	12.867684210913270
H	8.897549772759197	-1.890795551737068	14.251296865234920
H	4.715381910180513	3.197883352594816	13.551970064137558
H	6.125697045181663	2.477882035647999	13.300065339412305
H	6.910579760453339	-2.514226273214436	14.164708414686389
H	10.911393679561797	0.215167562032193	14.059963552869023
H	7.289491050871080	0.443523879050409	13.470798953798697
H	1.624285632539646	0.319506788839463	14.187595609431828
H	1.686270233908607	0.865421984602482	15.688014864042893

10.5. Low-energy c(2×2) structures

Structures for the low-energy c(2×2) surface reconstruction as displayed in **Figure 12**. Note that the structure for single H_2O adsorption is not shown in any figure.

Single H_2O adsorption

39

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	-0.400404017805987	3.197132022169984	12.226653994142788
Cu	-0.400403987628330	1.041216988399700	10.070739037261031
Cu	-2.555588996968988	5.352317001332985	12.226653994142788
Cu	-0.400404017805986	7.507501980495986	16.538483907906087
Cu	-0.400404017805987	3.197132022169984	16.538483907906087
Cu	-0.400403987628330	1.041216988399700	14.382568951024330
Cu	1.754781004467987	3.196401980496018	10.070739037261031
Cu	-2.555588996968988	5.352317001332985	16.538483907906087

Cu	-0.400404017805986	5.351587002769991	14.382568951024330
Cu	1.754781004467987	3.196401980496018	14.382568951024330
Cu	-2.555589009902304	3.196402010673674	14.382568951024330
Cu	1.754780961357015	5.352317001332985	16.538483907906087
Cu	-0.400404017805986	7.507501980495986	12.226653994142788
Cu	-0.400404017805986	5.351587002769991	10.070739037261031
Cu	-2.555589009902304	3.196402010673674	10.070739037261031
Cu	1.754780961357015	5.352317001332985	12.226653994142788
Cu	2.516673398461458	5.664848091251269	20.135249593275056
Cu	-0.247057623902916	1.221829788217892	18.237337333897241
Cu	0.787376250326443	1.021498020359574	20.338672119951639
Cu	-0.066556633311209	3.252325039216414	19.894186258422092
Cu	-0.789124953963334	7.630972354953016	20.123718625726120
Cu	-0.331572753109868	5.535245190621955	18.615325629941946
Cu	1.704587517064654	2.769716798772428	18.392229402568727
Cu	-2.510725307242497	3.396082404590689	18.720179461804463
O	-1.385217941358627	4.373126487894861	17.585846864580230
O	0.722678057717448	6.603337934639864	19.733983401209031
O	1.772577234271656	3.857377160799202	20.558863437139497
O	2.771424104830123	4.221994672172173	17.546592127859476
O	0.677553988388993	6.429543974301008	11.148696968444098
O	2.832738967551994	4.274358995138007	8.992782011562335
O	-1.477630990774009	4.274358995138006	13.304611925325640
O	0.677553988388993	6.429543974301008	15.460526882207397
O	2.832738967551994	4.274358995138007	13.304611925325640
O	-1.477630990774009	4.274358995138006	8.992782011562335
O	0.677553988388992	2.119174015975005	15.460526882207397

O	0.677553988388992	2.119174015975005	11.148696968444098
O	1.677228629835612	1.743636982245612	22.021379744376567
H	1.737992496289887	2.710542149222023	21.627119273157355
H	1.118915179551979	1.777257673126089	22.818855297545625

H_2O ML

48

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	-0.400404017805987	3.197132022169984	12.226653994142788
Cu	-0.400403987628330	1.041216988399700	10.070739037261031
Cu	-2.555588996968988	5.352317001332985	12.226653994142788
Cu	-0.400404017805986	7.507501980495986	16.538483907906087
Cu	-0.400404017805987	3.197132022169984	16.538483907906087
Cu	-0.400403987628330	1.041216988399700	14.382568951024330
Cu	1.754781004467987	3.196401980496018	10.070739037261031
Cu	-2.555588996968988	5.352317001332985	16.538483907906087
Cu	-0.400404017805986	5.351587002769991	14.382568951024330
Cu	1.754781004467987	3.196401980496018	14.382568951024330
Cu	-2.555589009902304	3.196402010673674	14.382568951024330
Cu	1.754780961357015	5.352317001332985	16.538483907906087
Cu	-0.400404017805986	7.507501980495986	12.226653994142788
Cu	-0.400404017805986	5.351587002769991	10.070739037261031
Cu	-2.555589009902304	3.196402010673674	10.070739037261031
Cu	1.754780961357015	5.352317001332985	12.226653994142788
Cu	1.868597518357652	5.718360635614423	20.333832355943667
Cu	-0.234528187524567	1.232050462609547	18.406978589532248
Cu	-2.791623942147061	5.529456618870396	20.112416885278765

Cu	-0.210797759929270	2.966491967823445	20.067404497757085
Cu	-0.567465923194246	8.040502142265884	20.416666183164875
Cu	-0.461753920980675	5.557707097259990	18.616337882679513
Cu	1.599553197974703	2.973607629479409	18.408778107112273
Cu	-2.542438281943734	3.391937984435132	18.599097117125375
O	-1.380729293190815	4.361906570934378	17.554017505053448
O	0.532101118150026	6.769739529727144	19.586342654391533
O	2.674910137832964	4.660187334411251	21.599087193955079
O	2.817971935442501	4.270994998908292	17.594068171830898
O	0.677553988388993	6.429543974301008	11.148696968444098
O	2.832738967551994	4.274358995138007	8.992782011562335
O	-1.477630990774009	4.274358995138006	13.304611925325640
O	0.677553988388993	6.429543974301008	15.460526882207397
O	2.832738967551994	4.274358995138007	13.304611925325640
O	-1.477630990774009	4.274358995138006	8.992782011562335
O	0.677553988388992	2.119174015975005	15.460526882207397
O	0.677553988388992	2.119174015975005	11.148696968444098
O	-0.758952201768274	6.824484746755264	23.212430200331042
O	-2.280765521640701	2.461324359680079	23.134848663773393
O	0.405773195944408	3.459791794170963	21.947811237742311
O	-2.248505126890183	5.099351910594399	21.967741331518180
H	3.342219413518896	3.380046736403611	22.777034387064880
H	0.231027526613335	6.756431617652089	23.226486405588339
H	-2.134655772619464	4.171326462442117	22.294013696718551
H	-1.558847364561966	5.696039552322675	22.435102983642032
H	-1.844437029523218	2.483290322344996	24.004445254431005
H	0.572973532585200	2.598167209978384	22.380603156687279

H	1.346749001234062	3.915959909122518	21.842643313590258
H	2.389090961974571	5.957942427009293	22.641080528302009

OH/H_2O ML

48

Lattice vectors: [4.316, 4.316, 0.000 ; -4.316, 4.316, 0.000 ; 0.000, 0.000, 34.528]

Cu	-0.400404017805987	3.197132022169984	12.226653994142788
Cu	-0.400403987628330	1.041216988399700	10.070739037261031
Cu	-2.555588996968988	5.352317001332985	12.226653994142788
Cu	-0.400404017805986	7.507501980495986	16.538483907906087
Cu	-0.400404017805987	3.197132022169984	16.538483907906087
Cu	-0.400403987628330	1.041216988399700	14.382568951024330
Cu	1.754781004467987	3.196401980496018	10.070739037261031
Cu	-2.555588996968988	5.352317001332985	16.538483907906087
Cu	-0.400404017805986	5.351587002769991	14.382568951024330
Cu	1.754781004467987	3.196401980496018	14.382568951024330
Cu	-2.555589009902304	3.196402010673674	14.382568951024330
Cu	1.754780961357015	5.352317001332985	16.538483907906087
Cu	-0.400404017805986	7.507501980495986	12.226653994142788
Cu	-0.400404017805986	5.351587002769991	10.070739037261031
Cu	-2.555589009902304	3.196402010673674	10.070739037261031
Cu	1.754780961357015	5.352317001332985	12.226653994142788
Cu	1.452391124202813	5.531636503255721	20.516642879256278
Cu	-0.210167469332714	1.264482741422360	18.403369400094242
Cu	-2.814152505941375	5.555078209643457	20.106927722200766
Cu	-0.083298223830820	3.096354853418601	20.058646700819754
Cu	3.589484055115618	3.595030847822705	20.429481669046545

Cu	-0.577413490332366	5.407201706768427	18.607575121959020
Cu	1.618146772509159	3.010466793221605	18.400383976915350
Cu	-2.712884774464240	3.291976744677635	18.600162996590456
O	-1.516424732551301	4.227380645167631	17.560185294044032
O	0.353644975393266	6.655846906933862	19.570555100009351
O	2.702583741277536	4.735183830782271	21.608233840203933
O	2.847883757772666	4.304056135423895	17.600088727755178
O	0.677553988388993	6.429543974301008	11.148696968444098
O	2.832738967551994	4.274358995138007	8.992782011562335
O	-1.477630990774009	4.274358995138006	13.304611925325640
O	0.677553988388993	6.429543974301008	15.460526882207397
O	2.832738967551994	4.274358995138007	13.304611925325640
O	-1.477630990774009	4.274358995138006	8.992782011562335
O	0.677553988388992	2.119174015975005	15.460526882207397
O	0.677553988388992	2.119174015975005	11.148696968444098
O	0.422853919028265	6.888375950505844	23.010878153531294
O	-0.632857463306194	3.134552166810297	21.930915161355347
O	1.516791029052943	2.909088003972993	23.264658320039889
O	-2.443500400699644	4.841898939304048	21.902763424713829
H	-0.526771731016359	7.035971258171641	23.180999622764713
H	0.762649425381639	7.761609222158610	22.704034541836236
H	-1.618482589230993	4.169618022623811	21.994342108325927
H	-2.416880688699112	5.585673216617543	22.558829781617174
H	0.588936061728625	3.031487366472701	22.771980319451973
H	1.359477576894938	3.095480219834384	24.206375871161683
H	2.251022112488589	4.182738827400197	22.303097014750648
H	-1.056203253230199	2.247512611994362	22.045705802370829