Electronic Supplementary Information (ESI) for:

Reactivity at the Cu$_2$O(100):Cu-H$_2$O Interface: A Combined DFT and PES study

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S1. Crystal structure and molecular optimization

1.1. The Cu$_2$O Crystal structure

Bulk Cu$_2$O adopts a cubic unit cell belonging to the Pn3 space group. The Cu$_2$O structure may be described as constructed by a face centered cubic (fcc) Cu sublattice and a body centered cubic (bcc) O sublattice, or, alternatively, as two intercalated fcc Cu$_2$O cristobalite-like sublattices. The initial crystal structure of Cu$_2$O was obtained from Werner et al, 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. 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$_2$O and H$_2$

The molecular gas phase calculations were 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, $H$, of the surface–adsorbate systems were considered. These were obtained numerically by displacing the atoms of the adsorbate and the top two Cu$_2$O layers $\pm 0.015$ 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$_2$O surfaces,$^{12}$ but generally only so if one is interested in relative energies and not of absolute energies. A mass-weighted Hessian, $H_{MW}$, 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 $H_{MW}$ 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 $H_{MW}$. This will generate three frequencies close to 0, and 3N-3 non-zero frequencies. The separation proceeds by transformation of the $H_{MW}$ into internal coordinates by:

$$H_{int} = D^\dagger H_{MW} D,$$

where the transformation matrix $D$ is the defined as the matrix that converts $q_{MW}$ into the internal coordinates $q_{int}$. $D$ is formed by:

$$D = I - d_1^t d_1 - d_2^t d_2 - d_3^t d_3$$

where the vector $d_1$, $d_2$ and $d_3$ are the mass-weighted and normalized translational vectors:

$$d'_1 = [\sqrt{m_1} 0 0 \sqrt{m_2} 0 0 \cdots \sqrt{m_N} 0 0]$$
$$d'_2 = [0 \sqrt{m_1} 0 0 \sqrt{m_2} 0 \cdots 0 \sqrt{m_N}]$$
$$d'_3 = [0 0 \sqrt{m_1} 0 0 \sqrt{m_2} \cdots 0 0 \sqrt{m_N}]$$

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

The vibrational frequencies can thereafter be obtained by diagonalizing $H_{int}$ and converting the resulting eigenvalues $\lambda_i$ to frequencies, $\nu_i$, by ($c$ is the speed of light):

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

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.

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, $\Delta G^\circ$, by

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

Assuming the study of an adsorption reaction, $\text{H}_2\text{O}(g) + S \rightarrow \text{H}_2\text{O-S} (\text{S=surface})$ and an initial standard state of 1 bar $\text{H}_2\text{O}$, the above relation yields the conversion factor $\Delta \Delta G^\circ \rightarrow \ast$ to an arbitrary $\text{H}_2\text{O}$ pressure $p_{\text{H}_2\text{O}}$:

$$\Delta \Delta G^\circ \rightarrow \ast = -RT\ln(p_{\text{H}_2\text{O}})$$

A similar relation is obtained for the conversion to an arbitrary $\text{H}_2$ pressure. The reaction Gibbs free energy for the new reference state, $\Delta G^\ast$, is obtained by adding $\Delta \Delta G^\circ \rightarrow \ast$ to the standard Gibbs free reaction energy $\Delta G^\circ$

$$\Delta G^\ast = \Delta G^\circ + \Delta \Delta G^\circ \rightarrow \ast$$

In order to convert to an aqueous state the conversion factor is, assuming a $\text{H}_2\text{O}$ concentration of 55 M ($0.041$ is the concentration of 1 bar of gaseous $\text{H}_2\text{O}$):

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

Note that the electronic energy, $E_{el}$, for $\text{H}_2\text{O}$ must be updated from $\text{H}_2\text{O}(g)$ to $\text{H}_2\text{O}(\text{aq})$ by inclusion of solvation effects. We have done so by adding standard PCM$^{16,17}$ corrections from Gaussian09$^{18}$ calculations on monomer $\text{H}_2\text{O}$. 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$_2$O/OH/H$_2$ adsorption/dissociation states on the ridge-dimer c(2×2) reconstructed Cu$_2$O(100):Cu surface. Reprints from Figure 7 in the main article.

<table>
<thead>
<tr>
<th>State$^a$</th>
<th>$\Delta E_{el}$</th>
<th>$\Delta H$</th>
<th>$\Delta G$</th>
<th>$\Delta H$</th>
<th>$\Delta H$</th>
<th>$\Delta H$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$^{PBE-D3+U}$</td>
<td>$^{PBE-D3+U}$</td>
<td>$^{PBE-D3+U}$</td>
<td>$^{PBE}$</td>
<td>$^{PBE-D3}$</td>
<td>$^{HSE06-D3}$</td>
</tr>
<tr>
<td>1-H$_2$O 0/4</td>
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<td>-0.60</td>
<td>-0.10</td>
<td>-0.33</td>
<td>-0.57</td>
<td>-0.59</td>
</tr>
<tr>
<td>1-H$_2$O 1/4*</td>
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<td>-2.19</td>
<td>-1.66</td>
<td>-1.93</td>
<td>-2.09</td>
<td>-2.80</td>
</tr>
<tr>
<td>1-H$_2$O 1/4</td>
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<td>-0.79</td>
<td>-0.98</td>
<td>-1.08</td>
<td>-1.48</td>
</tr>
<tr>
<td>2-H$_2$O 0/4</td>
<td>-1.28</td>
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<td>-0.21</td>
<td>-0.82</td>
<td>-1.18</td>
<td>-1.14</td>
</tr>
<tr>
<td>2-H$_2$O 1/4*</td>
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<td>-1.74</td>
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<td>-2.61</td>
<td>-3.28</td>
</tr>
<tr>
<td>2-H$_2$O 2/4*</td>
<td>-0.55</td>
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<td>0.40</td>
<td>-0.37</td>
<td>-0.81</td>
<td>-0.46</td>
</tr>
<tr>
<td>2-H$_2$O 1/4</td>
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<td>-1.79</td>
<td>-0.95</td>
<td>-1.41</td>
<td>-1.68</td>
<td>-2.04</td>
</tr>
<tr>
<td>2-H$_2$O 2/4</td>
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<td>-2.38</td>
<td>-1.68</td>
<td>-1.98</td>
<td>-2.20</td>
<td>-3.01</td>
</tr>
<tr>
<td>3-H$_2$O 0/4</td>
<td>-2.36</td>
<td>-2.16</td>
<td>-0.71</td>
<td>-1.55</td>
<td>-2.15</td>
<td>-2.26</td>
</tr>
<tr>
<td>3-H$_2$O 1/4*</td>
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<td>-3.42</td>
<td>-1.99</td>
<td>-2.72</td>
<td>-3.28</td>
<td>-4.00</td>
</tr>
<tr>
<td>3-H$_2$O 1/4</td>
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<td>-2.06</td>
<td>-2.56</td>
<td>-3.01</td>
</tr>
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<td>-3.01</td>
<td>-3.93</td>
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<tr>
<td>3-H$_2$O 3/4</td>
<td>-1.44</td>
<td>-1.65</td>
<td>-0.60</td>
<td>-1.20</td>
<td>-1.56</td>
<td>-1.48</td>
</tr>
<tr>
<td>4-H$_2$O 0/4</td>
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<td>-2.56</td>
<td>-0.60</td>
<td>-1.66</td>
<td>-2.52</td>
<td>-2.43</td>
</tr>
<tr>
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<td>-1.44</td>
<td>-2.62</td>
<td>-3.29</td>
<td>-3.87</td>
</tr>
<tr>
<td>4-H$_2$O 1/4</td>
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<td>-1.97</td>
<td>-2.64</td>
<td>-2.84</td>
</tr>
<tr>
<td>4-H$_2$O 2/4</td>
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<td>-3.07</td>
<td>-1.36</td>
<td>-2.30</td>
<td>-2.86</td>
<td>-3.61</td>
</tr>
<tr>
<td>4-H$_2$O 3/4</td>
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<td>-1.89</td>
<td>-0.35</td>
<td>-1.24</td>
<td>-1.84</td>
<td>-1.76</td>
</tr>
<tr>
<td>4-H$_2$O 4/4</td>
<td>-0.68</td>
<td>-0.98</td>
<td>0.43</td>
<td>-0.42</td>
<td>-0.93</td>
<td>0.11</td>
</tr>
</tbody>
</table>

$^a$Degree of dissociation, $x$OH per surface Cu. The asterisk (*) marks $\text{H}_\text{ad}$ as dissociation product rather than $\text{H}_2(\text{g})$. 
Table S2. Energies in eV for the p(2×2) surface unit cell compared to the c(2×2) unit cell for the various H₂O/OH/H adsorption/dissociation states on the ridge-dimer c(2×2) reconstructed Cu₂O(100):Cu surface. Reprints from Figure 9 in the main article.

<table>
<thead>
<tr>
<th>State</th>
<th>ΔH</th>
<th>ΔG</th>
<th>ΔH</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>p(2×2)</td>
<td>p(2×2)</td>
<td>c(2×2)</td>
</tr>
<tr>
<td>0/8</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>1/8*</td>
<td>-1.07</td>
<td>-1.03</td>
<td>-0.89</td>
</tr>
<tr>
<td>1/8</td>
<td>-0.39</td>
<td>-0.48</td>
<td>-0.20</td>
</tr>
<tr>
<td>2/8*</td>
<td>-1.74</td>
<td>-1.62</td>
<td>-1.78</td>
</tr>
<tr>
<td>2/8</td>
<td>-0.36</td>
<td>-0.59</td>
<td>-0.40</td>
</tr>
<tr>
<td>3/8*</td>
<td>0.04</td>
<td>0.13</td>
<td>(-)</td>
</tr>
<tr>
<td>3/8</td>
<td>-0.78</td>
<td>-1.20</td>
<td>-0.71</td>
</tr>
<tr>
<td>4/8*</td>
<td>2.36</td>
<td>2.63</td>
<td>(-)</td>
</tr>
<tr>
<td>4/8</td>
<td>-0.97</td>
<td>-1.46</td>
<td>-1.03</td>
</tr>
<tr>
<td>5/8</td>
<td>0.23</td>
<td>-0.43</td>
<td>0.15</td>
</tr>
<tr>
<td>6/8</td>
<td>1.41</td>
<td>0.56</td>
<td>1.33</td>
</tr>
<tr>
<td>7/8</td>
<td>2.45</td>
<td>1.45</td>
<td>2.24</td>
</tr>
<tr>
<td>8/8</td>
<td>3.32</td>
<td>2.22</td>
<td>3.16</td>
</tr>
</tbody>
</table>

*Degree of dissociation, xOH per surface Cu. The asterisk (*) marks H₂(g) as dissociation product rather than H₂(g).
Table S3. Energies in eV for bilayer (BL) and monolayer (ML) adsorption for the various H$_2$O/OH/H adsorption/dissociation states using the c(2×2) unit cell on the ridge-dimer c(2×2) reconstructed Cu$_2$O(100):Cu surface. Reprints from Figure 11 in the main article.

<table>
<thead>
<tr>
<th>State $^a$</th>
<th>$\Delta H$</th>
<th>$\Delta G$</th>
<th>$\Delta H$</th>
<th>$\Delta G$</th>
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<tr>
<td></td>
<td>ML</td>
<td>BL</td>
<td>ML</td>
<td>BL</td>
</tr>
<tr>
<td>0/4</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>1/4$^*$</td>
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<td>-1.03</td>
<td>-0.84</td>
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<td>-0.65</td>
</tr>
<tr>
<td>2/4</td>
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<td>-0.77</td>
<td>-0.76</td>
<td>-1.00</td>
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<td>3/4</td>
<td>0.66</td>
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<td>0.25</td>
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<tr>
<td>4/4</td>
<td>1.58</td>
<td>1.06</td>
<td>1.03</td>
<td>0.50</td>
</tr>
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</table>

$^a$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 Cu₂O(100):Cu surface converted to realistic humid and wet conditions at 298.15 K. The case of standard 1 bar H₂O partial pressure, as used in the main article, is included for comparison.

<table>
<thead>
<tr>
<th></th>
<th>22% RH</th>
<th>100% RH</th>
<th>1 bar</th>
<th>55ML</th>
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<tr>
<td>1-H₂O</td>
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<tr>
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<td>0.03</td>
<td>-0.01</td>
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<td>-0.05</td>
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<tr>
<td>1-H₂O</td>
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<td></td>
</tr>
<tr>
<td>1/4*</td>
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<td>-1.57</td>
<td>-1.66</td>
<td>-1.61</td>
</tr>
<tr>
<td>1-H₂O</td>
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<td></td>
</tr>
<tr>
<td>1/4</td>
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<td>-0.70</td>
<td>-0.79</td>
<td>-0.74</td>
</tr>
<tr>
<td>2-H₂O</td>
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</tr>
<tr>
<td>0/4</td>
<td>0.05</td>
<td>-0.03</td>
<td>-0.21</td>
<td>-0.10</td>
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<tr>
<td>2-H₂O</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>1/4*</td>
<td>-1.49</td>
<td>-1.57</td>
<td>-1.74</td>
<td>-1.64</td>
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<tr>
<td>2-H₂O</td>
<td></td>
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<tr>
<td>2/4*</td>
<td>0.66</td>
<td>0.58</td>
<td>0.40</td>
<td>0.51</td>
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<tr>
<td>2-H₂O</td>
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<tr>
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<td>2-H₂O</td>
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<tr>
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<td>-1.50</td>
<td>-1.68</td>
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<td>3-H₂O</td>
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<td>3-H₂O</td>
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<td>-1.39</td>
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<td>3-H₂O</td>
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<td>4-H₂O</td>
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<td>1/4*</td>
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<td>-1.09</td>
<td>-1.44</td>
<td>-1.23</td>
</tr>
<tr>
<td>4-H₂O</td>
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</tr>
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<tr>
<td>4-H₂O</td>
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</tr>
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<td>-0.85</td>
<td>-1.01</td>
<td>-1.36</td>
<td>-1.15</td>
</tr>
<tr>
<td>4-H₂O</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3/4</td>
<td>0.16</td>
<td>0.00</td>
<td>-0.35</td>
<td>-0.14</td>
</tr>
<tr>
<td>4-H₂O</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4/4</td>
<td>0.94</td>
<td>0.79</td>
<td>0.43</td>
<td>0.64</td>
</tr>
</tbody>
</table>

*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 H₂-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 Cu₂O(100):Cu surface converted to different H₂ partial pressures. Wet conditions (i.e. 55 ML H₂O) have been assumed.

<table>
<thead>
<tr>
<th></th>
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<th>1 mbar</th>
<th>531 nbar</th>
<th>1 fbar</th>
</tr>
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<tbody>
<tr>
<td>1-H₂O</td>
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<td>-0.05</td>
<td>-0.05</td>
</tr>
<tr>
<td>1-H₂O</td>
<td>1/4*</td>
<td>-1.61</td>
<td>-1.61</td>
<td>-1.61</td>
</tr>
<tr>
<td>1-H₂O</td>
<td>1/4</td>
<td>-0.55</td>
<td>-0.64</td>
<td>-0.74</td>
</tr>
<tr>
<td>2-H₂O</td>
<td>0/4</td>
<td>-0.10</td>
<td>-0.10</td>
<td>-0.10</td>
</tr>
<tr>
<td>2-H₂O</td>
<td>1/4*</td>
<td>-1.64</td>
<td>-1.64</td>
<td>-1.64</td>
</tr>
<tr>
<td>2-H₂O</td>
<td>2/4*</td>
<td>0.51</td>
<td>0.51</td>
<td>0.51</td>
</tr>
<tr>
<td>2-H₂O</td>
<td>1/4</td>
<td>-0.66</td>
<td>-0.75</td>
<td>-0.85</td>
</tr>
<tr>
<td>2-H₂O</td>
<td>2/4</td>
<td>-1.20</td>
<td>-1.38</td>
<td>-1.57</td>
</tr>
<tr>
<td>3-H₂O</td>
<td>0/4</td>
<td>-0.55</td>
<td>-0.55</td>
<td>-0.55</td>
</tr>
<tr>
<td>3-H₂O</td>
<td>1/4*</td>
<td>-1.83</td>
<td>-1.83</td>
<td>-1.83</td>
</tr>
<tr>
<td>3-H₂O</td>
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<td>-1.04</td>
<td>-1.13</td>
<td>-1.23</td>
</tr>
<tr>
<td>3-H₂O</td>
<td>2/4</td>
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<td>-1.69</td>
<td>-1.88</td>
</tr>
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<td>3-H₂O</td>
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<td>0.12</td>
<td>-0.15</td>
<td>-0.44</td>
</tr>
<tr>
<td>4-H₂O</td>
<td>0/4</td>
<td>-0.39</td>
<td>-0.39</td>
<td>-0.39</td>
</tr>
<tr>
<td>4-H₂O</td>
<td>1/4*</td>
<td>-1.23</td>
<td>-1.23</td>
<td>-1.23</td>
</tr>
<tr>
<td>4-H₂O</td>
<td>1/4</td>
<td>-0.51</td>
<td>-0.60</td>
<td>-0.70</td>
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<td>4-H₂O</td>
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<td>-1.15</td>
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<td>4-H₂O</td>
<td>3/4</td>
<td>0.42</td>
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<tr>
<td>4-H₂O</td>
<td>4/4</td>
<td>1.38</td>
<td>1.03</td>
<td>0.64</td>
</tr>
</tbody>
</table>

*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$_2$O 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$_2$O adsorption at the favored site is shown in Figure S2 and the ML structure for the OH/H$_2$O ML with the OH:H$_2$O ratio of 1:5 is shown in Figure S3.

Table S6. Adsorption energies in eV/H$_2$O for the (3,0;1,1) surfaces. Energies are given as electronic energy without thermal corrections. Adsorption sites are specified in Figure S1.

<table>
<thead>
<tr>
<th>Surface</th>
<th>Site/mode</th>
<th>$E_{ad}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3,0;1,1)</td>
<td>1$^{a,b)}$</td>
<td>-0.24</td>
</tr>
<tr>
<td></td>
<td>2$^{a,e)}$</td>
<td>-0.27</td>
</tr>
<tr>
<td></td>
<td>3$^{a,e)}$</td>
<td>-0.56</td>
</tr>
<tr>
<td></td>
<td>4$^{a,b)}$</td>
<td>-0.66</td>
</tr>
<tr>
<td></td>
<td>5$^{c,e)}$</td>
<td>-0.42</td>
</tr>
<tr>
<td></td>
<td>6$^{a,f)}$</td>
<td>-0.70</td>
</tr>
<tr>
<td></td>
<td>7$^{a,g)}$</td>
<td>-0.53</td>
</tr>
<tr>
<td>H$_2$O ML</td>
<td></td>
<td>-0.55</td>
</tr>
<tr>
<td>OH/H$_2$O ML</td>
<td></td>
<td>-0.65</td>
</tr>
</tbody>
</table>

$^a$) 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$_2$O 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$_{\text{bulk}}$ (●), Cu$_{\text{surf}}$ (▲), O$_{\text{bulk}}$ (◆) and O$_{\text{surf}}$ (○).

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

Figure S3. H$_2$O/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.

<table>
<thead>
<tr>
<th>Surface site</th>
<th>$E_{ad}$ [eV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A1$</td>
<td>-0.38</td>
</tr>
<tr>
<td>$A2$</td>
<td>-0.51</td>
</tr>
<tr>
<td>$A3$</td>
<td>-0.72 (-0.97)</td>
</tr>
<tr>
<td>$A4$</td>
<td>-0.60</td>
</tr>
<tr>
<td>$B1$</td>
<td>-0.32</td>
</tr>
<tr>
<td>$B2$</td>
<td>-0.39</td>
</tr>
<tr>
<td>$B3$</td>
<td>-0.43</td>
</tr>
<tr>
<td>$B4$</td>
<td>-0.69</td>
</tr>
<tr>
<td>$B5$</td>
<td>-0.57</td>
</tr>
<tr>
<td>$H1$</td>
<td>-0.35</td>
</tr>
<tr>
<td>$H2$</td>
<td>-0.53</td>
</tr>
<tr>
<td>$H3$</td>
<td>-0.43</td>
</tr>
</tbody>
</table>

---

a) H$_2$O 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$_2$O layers and the interacting H$_2$O.
Figure S4. Depicts H$_2$O adsorption sites for the low-energy reconstructed c(2×2) surface. Coloring: Cu(●), O (●) and H (○).

6.3. H$_2$O monolayer on the ridge-dimer c(2×2) using the p(2×2) unit cell

Figure S5. Shows the H$_2$O 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$_2$O adsorption processes reveal strong cooperative effects upon binding to the Cu$_2$O(100):Cu surface, especially at intermediate H$_2$O 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\textsuperscript{19} the desorption of a H\textsubscript{2}O covered Cu\textsubscript{2}O(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\textsubscript{2}O decreases with the H\textsubscript{2}O 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\textsubscript{2}O dissociation on the surface, the adsorption study was repeated using a p(2×2) surface unit cell and Cu\textsubscript{2}(100):Cu-(OH/H)\textsubscript{(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$_2$O(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$_2$O(100):Cu + H$_2$O(g) $\rightarrow$ Cu$_2$O(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 1 ML 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)\textsuperscript{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$_2$O 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$_2$O 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 (Cu₂O)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, employing the PBE₀²⁴-D³ₓ-c functional, the split-J²⁵ def2-SVP/J basis set²⁶–²⁸ 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.³²
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 differences from the 2L case.

Table S8. Convergence test for critical computational parameters: i) number of K-points, ii) plane-wave cut-off and iii) vacuum 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.

<table>
<thead>
<tr>
<th>K-points</th>
<th>$E_{ad}(H_2O)$</th>
<th>Cut-off</th>
<th>$E_{ad}(H_2O)$</th>
<th>Vacuum</th>
<th>$E_{ad}(H_2O)$</th>
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</thead>
<tbody>
<tr>
<td>2×2×1</td>
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<td>320 eV</td>
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<tr>
<td>4×4×1</td>
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<td>400 eV</td>
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<tr>
<td>8×8×1</td>
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<tr>
<td></td>
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<td>800 eV</td>
<td>-0.66</td>
<td>17 Å$^a$</td>
<td>-0.66</td>
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</tbody>
</table>

$^a$ 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 Cu₂O layers unconstraint during the geometrical relaxation.

<table>
<thead>
<tr>
<th>State</th>
<th>2L</th>
<th>4L</th>
</tr>
</thead>
<tbody>
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<td>1-H₂O 0/4</td>
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<td>-0.66</td>
</tr>
<tr>
<td>1-H₂O 1/4*</td>
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<td>-2.18</td>
</tr>
<tr>
<td>1-H₂O 1/4</td>
<td>-1.11</td>
<td>-1.12</td>
</tr>
<tr>
<td>2-H₂O 0/4</td>
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<td>-1.28</td>
</tr>
<tr>
<td>2-H₂O 1/4*</td>
<td>-2.80</td>
<td>-2.79</td>
</tr>
<tr>
<td>2-H₂O 2/4*</td>
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<td>-0.53</td>
</tr>
<tr>
<td>2-H₂O 1/4</td>
<td>-1.81</td>
<td>-1.82</td>
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<td>-2.25</td>
</tr>
<tr>
<td>3-H₂O 0/4</td>
<td>-2.36</td>
<td>-2.35</td>
</tr>
<tr>
<td>3-H₂O 1/4*</td>
<td>-3.57</td>
<td>-3.56</td>
</tr>
<tr>
<td>3-H₂O 1/4</td>
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<td>-3.19</td>
<td>-3.17</td>
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<tr>
<td>4-H₂O 0/4</td>
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<td>4-H₂O 1/4</td>
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<tr>
<td>4-H₂O 4/4</td>
<td>-0.68</td>
<td>-0.69</td>
</tr>
</tbody>
</table>

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 from the NIST Electron Inelastic-Mean-Free-Path Database. 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 \( E_{g}^{\text{Cu}_2\text{O}} = 2.2 \text{ eV} \), \( E_{g}^{\text{H}_2\text{O}} = 7.0 \text{ eV} \), density \( \rho^{\text{Cu}_2\text{O}} = 6 \text{ g cm}^{-3} \), \( \rho^{\text{H}_2\text{O}} = 0.9971 \text{ g cm}^{-3} \), and the number of valence electrons \( N_{v}^{\text{Cu}_2\text{O}} = 28 \), \( N_{v}^{\text{H}_2\text{O}} = 8 \). The resulting mean free paths at 120 eV kinetic energy are \( \lambda^{\text{Cu}_2\text{O}} = 5.37 \text{ Å} \) for \( \text{Cu}_2\text{O} \) and \( \lambda^{\text{H}_2\text{O}} = 8.65 \text{ Å} \) for \( \text{H}_2\text{O} \). The inelastic mean free path of \( \text{OH} \) was assumed to be equal to that of \( \text{H}_2\text{O} \). The thickness of a monolayer of hydroxyl groups was defined using the DFT geometry from the present study for \( \text{OH} \) adsorbed on \( \text{Cu}_2\text{O}(100) \), 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. The calculated thicknesses of the \( \text{OH} \) and \( \text{H}_2\text{O} \) layers were converted into monolayer coverage by dividing by their respective layer thickness. The coverage of \( \text{H}_2\text{O} \) and \( \text{OH} \) was estimated from their fraction of the intensity of the integrated O 1s intensity. A layered structure was assumed in the simulations with \( \text{H}_2\text{O} \) adsorbed closest to the vacuum and \( \text{OH} \) at the \( \text{Cu}_2\text{O} \) interface. The photoelectron contributions from the \( \text{H}_2\text{O} \) and \( \text{OH} \) layers as well as from a \( \text{Cu}_2\text{O} \) 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


(20) Glendening, E. D.; Reed, A. E.; Carpenter, J. E.; Weinhold, F. The NBO 3.0 Program Manual


### 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$_2$O coverage – 0/4 OH

<table>
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<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
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</tr>
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</tr>
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</tr>
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<td>16.5384799999999911</td>
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</tr>
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### 0.25 ML H$_2$O coverage – 1/4 OH

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

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0.50 ML H₂O coverage – 0/4 OH

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### 0.50 ML H₂O coverage – 1/4* OH

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0.50 ML H$_2$O coverage – 1/4 OH

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**0.50 ML H$_2$O 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]

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0.50 ML H₂O coverage – 2/4 OH

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

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Cu  -2.558494685811035      5.358403451555297     12.226650000000033
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Cu  -0.400855094987373      5.357672621836652     14.382569999999925
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Cu   1.756774484470320      5.358403451555267     16.538479999999911
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0.75 ML H₂O coverage – 0/4 OH

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

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Cu  -2.189641687546193  4.172143809706766  13.529181908835975
Cu  -0.064895365627976  6.202807662616213  13.447984958063564
Cu    0.093074574031842  8.153718352523001  15.091785767920459
Cu    2.288694793816049  2.460170807408186  15.105778579597555
Cu    2.253992873073093  4.424018037647317  13.579413887849562
Cu    0.116006879146529  2.225744638795727  13.664150710678898
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Cu    1.786870593813765  6.500129234204579  15.13000812455308
Cu    2.157994995164452  6.473994995164452  11.467750000000004
Cu    0.000000000000000  0.000000000000000  11.467750000000004
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O   -3.236762126534094  2.337122467363394  8.248378516994340
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O   -0.933557947886833  1.14368232057414  4.754355880643406
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0.75 ML H$_2$O 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]

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**0.75 ML H₂O coverage – 1/4 OH**

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### 0.75 ML H₂O coverage – 2/4 OH

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O 1.181763961549831 3.286330359110539 16.68070548737904
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0.75 ML H₂O coverage – 3/4 OH

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Cu 1.756774484470320 3.200033031012960 10.070740000000047
Cu -2.558494685811035 5.358403451555297 16.538479999999911
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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
1.00 ML H₂O coverage – 0/4 OH

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

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1.00 ML H₂O coverage – 1/4* OH

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1.00 ML H$_2$O coverage – 1/4 OH

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1.00 ML H$_2$O coverage – 2/4 OH

46

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**1.00 ML H$_2$O coverage – 3/4 OH**

45

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1.00 ML H₂O coverage – 4/4 OH

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The H$_2$O monolayer structure displayed in Figure 10 of the main article and in Figure S5:

### 0.25 ML H$_2$O coverage – 0/4 OH

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### 10.3. Double-layer structures

Structures displayed in Figure 11 of the main article.

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#### 0/4 OH

60

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**1/4* OH**

60

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

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### 1/4 OH

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Lattice vectors: $[4.316, 4.316, 0.000; -4.316, 4.316, 0.000; 0.000, 0.000, 34.528]$
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2/4 OH

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

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3/4 OH

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

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### 4/4 OH

56

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### 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$_2$O adsorption**

57

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

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### 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$_2$O adsorption is not shown in any figure.

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48

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