Supporting Information for "Interface Modeling for the *Ab Initio* Evaluation of the Water Contact Angle on a Metallic Cu(111) Surface"

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All the structures we used in the calculations are provided in xsf-format, as well as in figures shown below.

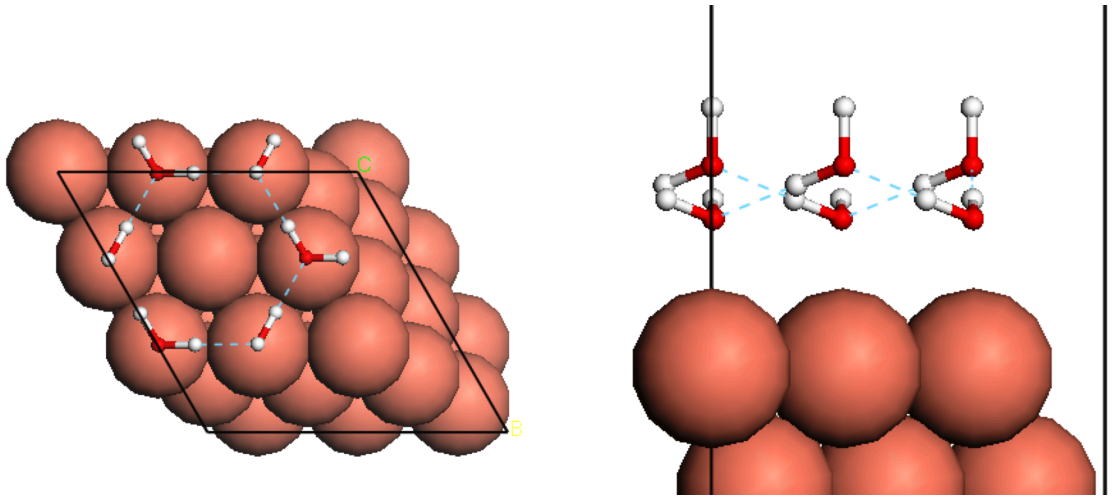

Figure S 1. Atomic geometry of the ice-like bilayer structure (left:topview, right:sideview). Cu atoms (bigger red balls) form a 3×3 unitcell, on which six H_2O molecules are located with the on-top geometry.

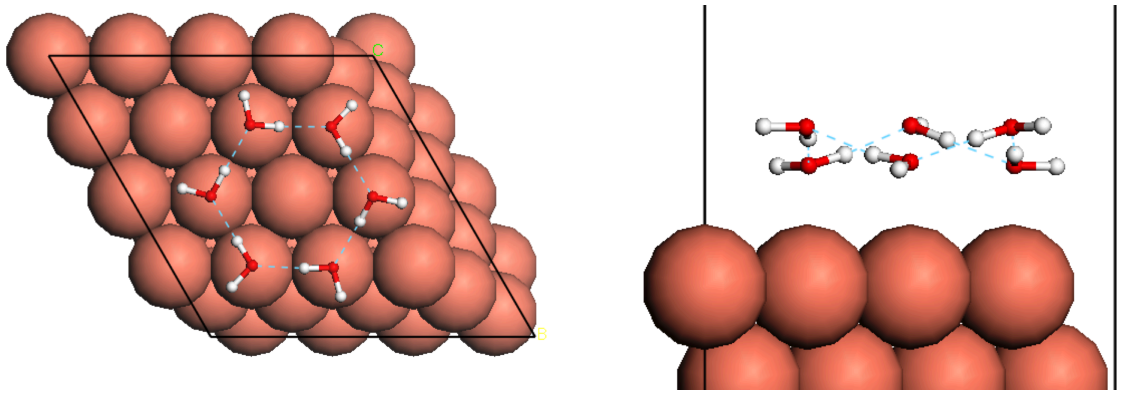

Figure S 2. Atomic geometry of the cyclic structure (buckled) for the water hexamer (left:topview, right:sideview). Cu atoms (bigger red balls) form a 4×4 unitcell, on which six H_2O molecules are located with the on-top geometry. Adjacent molecules take the vertical height difference of each oxygen site being ~0.85Å.

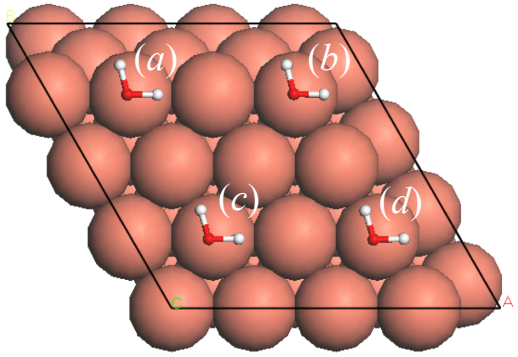

Figure S 3. Atomic geometry of the monomer adsorption model (topview) on Cu(111) surface (Cu atoms shown as bigger red balls). H_2O molecules are located with the on-top geometry. We considered four-molecule configuration (as shown in the picture), as well as three- [by putting molecules at (a),(b),(c)], two- [at (b),(c)], and one-molecule configuration [only at (c)], corresponding to the variation of coverage.

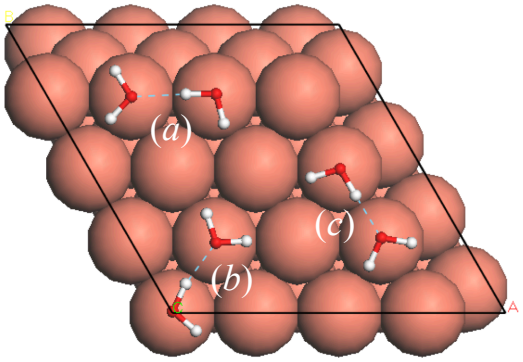

Figure S 4. Atomic geometry of the dimer adsorption model (topview) on Cu(111) surface (Cu atoms shown as bigger red balls). H_2O molecules are located with the on-top geometry. We considered three-cluster configuration (as shown in the picture), as well as two- [by putting clusters at (a),(b)], and one-cluster configuration [only at (b)], corresponding to the variation of coverage.

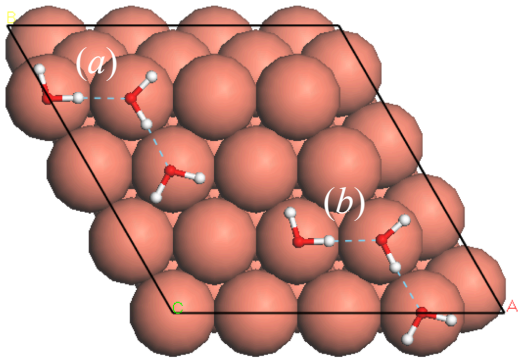

Figure S 5. Atomic geometry of the trimer (chain) adsorption model (topview) on Cu(111) surface (Cu atoms shown as bigger red balls). H_2O molecules are located with the on-top geometry. We considered two-cluster configuration (as shown in the picture), as well as one-cluster configuration [by putting the cluster only at (a)], corresponding to the variation of coverage.

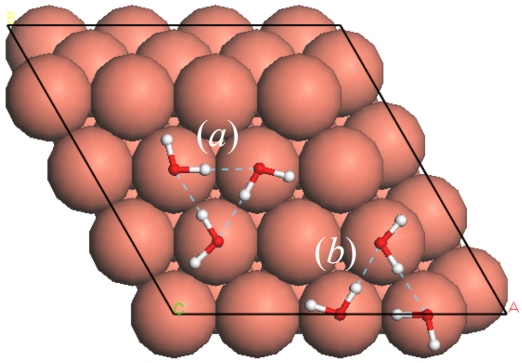

Figure S 6. Atomic geometry of the trimer (cyclic) adsorption model (topview) on Cu(111) surface (Cu atoms shown as bigger red balls). H_2O molecules are located with the on-top geometry. We considered two-cluster configuration (as shown in the picture), as well as one-cluster configuration [by putting the cluster only at (a)], corresponding to the variation of coverage.

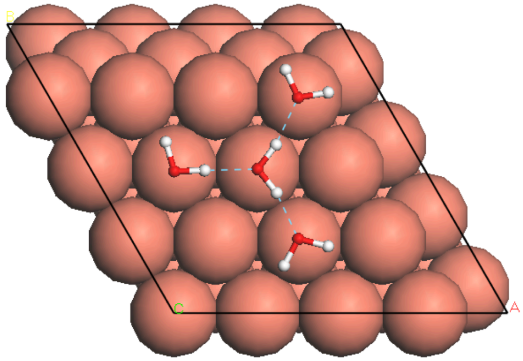

Figure S 7. Atomic geometry of the tetramer (chain) adsorption model (topview) on Cu(111) surface (Cu atoms shown as bigger red balls). H_2O molecules are located with the on-top geometry.

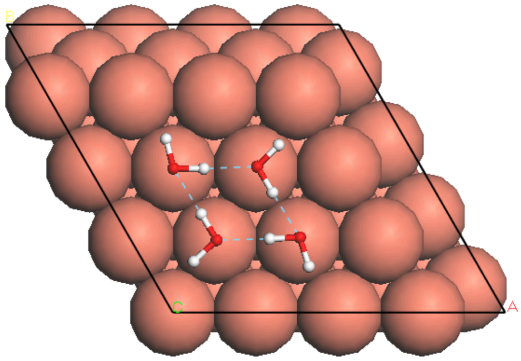

Figure S 8. Atomic geometry of the tetramer (cyclic) adsorption model (topview) on Cu(111) surface (Cu atoms shown as bigger red balls). H_2O molecules are located with the on-top geometry.

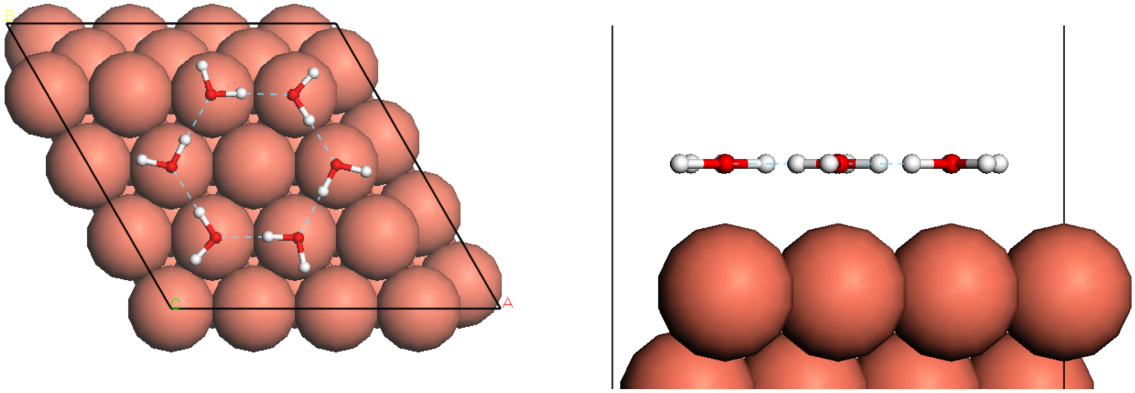

Figure S 9. Atomic geometry of the hexamer (cyclic/planar) adsorption model (left:topview, right:sideview) on Cu(111) surface (Cu atoms shown as bigger red balls). H_2O molecules are located with the on-top geometry.