Supplementary Information

Oriented Attachment Growth of Monocrystalline Cuprous Oxide Nanowires in Pure Water

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Contents

adsorption. (a) Side and top view of the fully relaxed (3×3) Cu_2O(100):O surface. (b) Side and top views of the configurations of the configuration with a water molecule adsorbed on the fully relaxed (3×3) Cu_2O(100):O surface. (c) and (d) present the fully relaxed structure of (3×2) Cu_2O(110):CuO surface and the stable configuration with a water molecule, top and side views are shown. (e) and (f) are the fully relaxed configurations of (2×2) Cu_2O(111):O surface and the stable structure with a water molecule adsorbed, top and side views are shown.

Figure S10. The stable configurations of a water molecule adsorbed on (a) (1×1) Cu_2O(100):O surface, (b) (1×1) Cu_2O(110):CuO surface and (c) (1×1) Cu_2O(111):O surface.

Figure S11. Fitted parameters and curves of the entropy of liquid water. The fitting data are from NIST-JANAF Thermochemical TABLEs (http://kinetics.nist.gov/janaf/).

Characterization details.

Reference

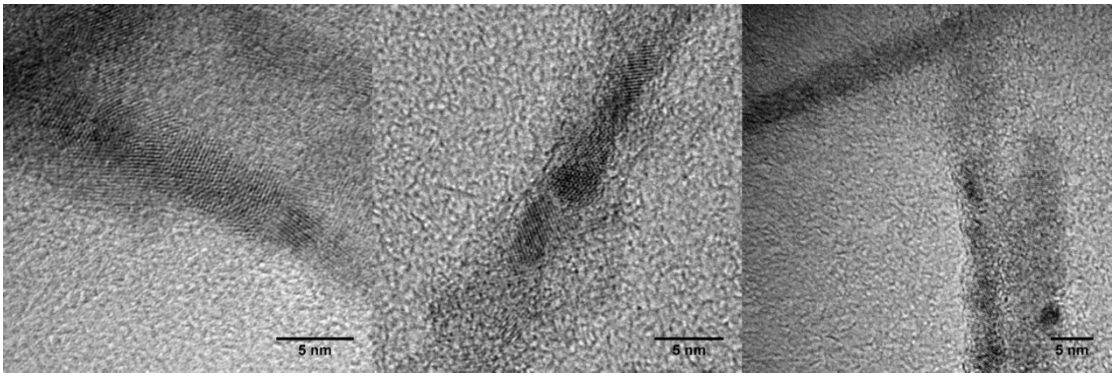

Figure S1. HRTEM images of the polycrystalline nanowires of Cu_2O synthesized at 25℃. Images were taken using FEI Tecnai T20 G^2. Random coalescence of crystals is clearly seen.

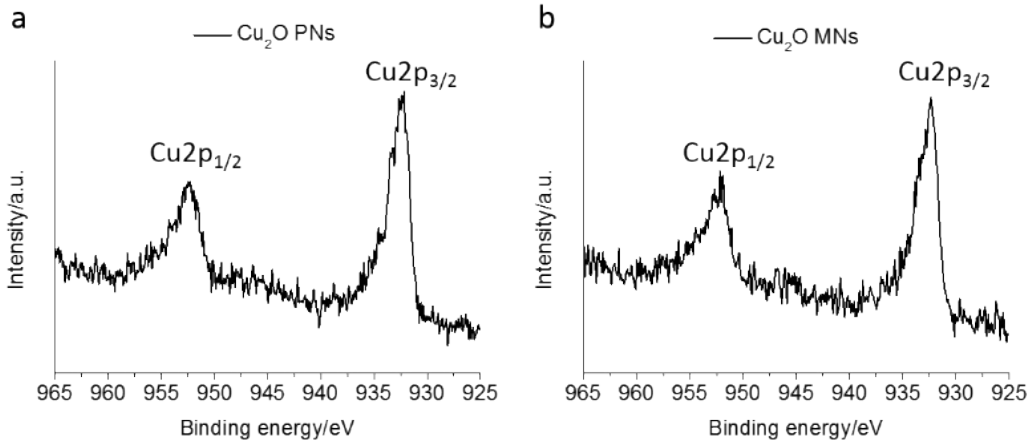

Figure S2. XPS spectra of Cu_2O nanowires synthesized (a) at 25℃ and (b) at 90℃.

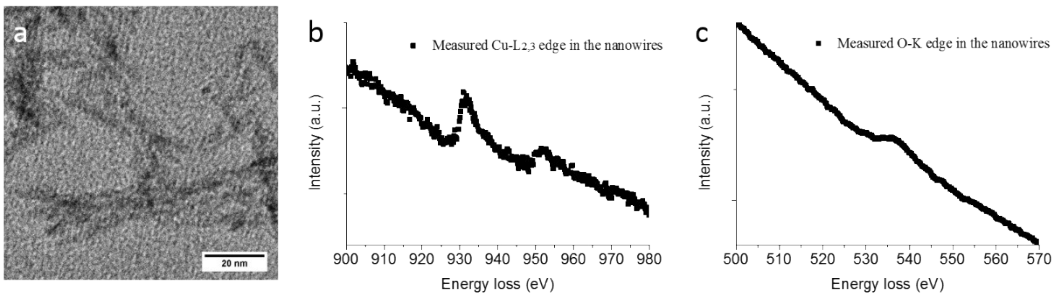

Figure S3. TEM image (a) and corresponding EELS spectra of Cu-L2, 3 (b) and O-K (c) edges measured in Cu_2O nanowires synthesized at 90℃. The features and positions of Cu-L2, 3 peaks and O-K peak match well with those for cuprous oxide.[1]

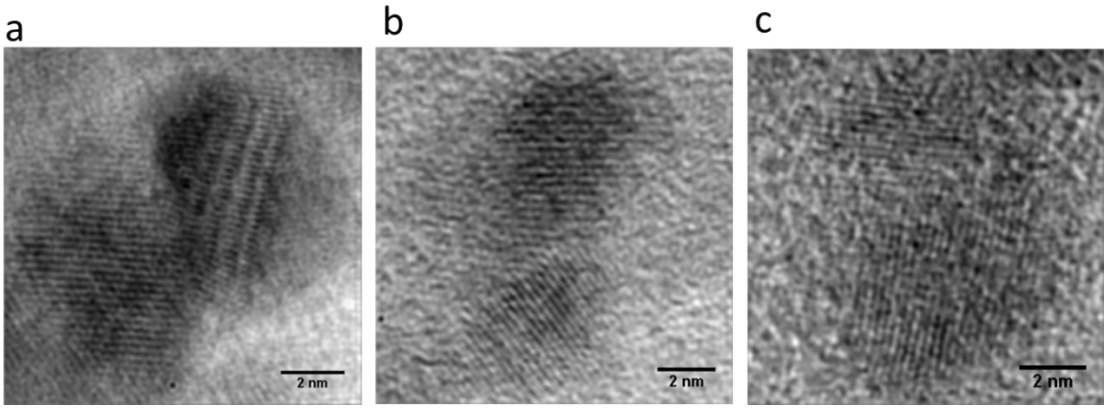

Figure S4. The initial transient of coalescence of two Cu_2O nanocrystals synthesized at 90℃.

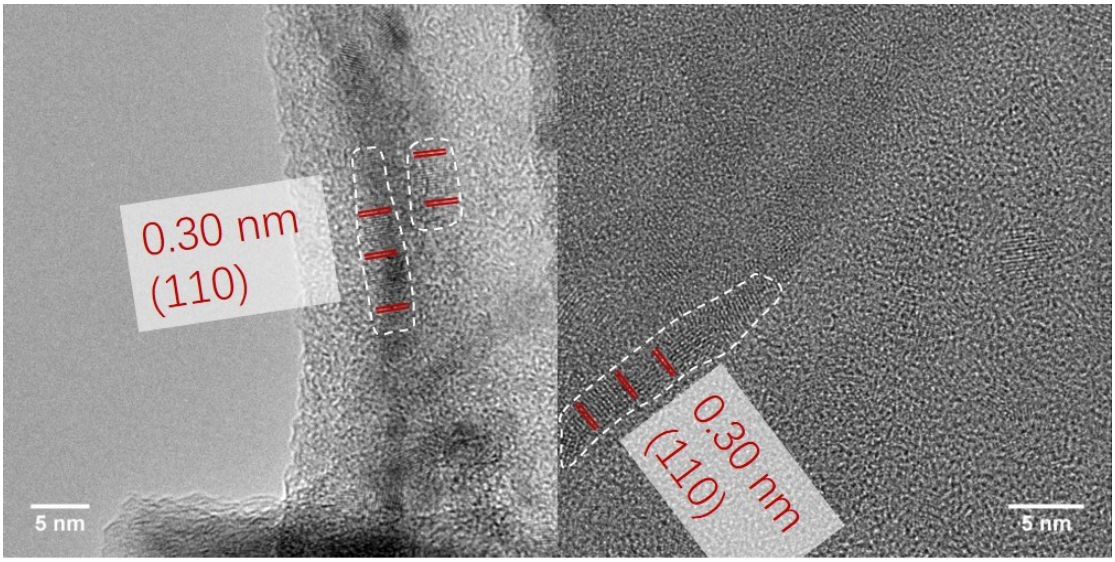

Figure S5. HRTEM images of the monocrystalline nanowires of Cu_2O synthesized at 90℃. The left panel was taken using FEI Tecnai T20 G^2. The right panel was taken using FEI Titan E-Cell 80-300 ST TEM. Even the nanowires were damaged more or less by the electron beam irradiation, the fragments as indicated could clearly show the oriented attachment of nanocrystals.

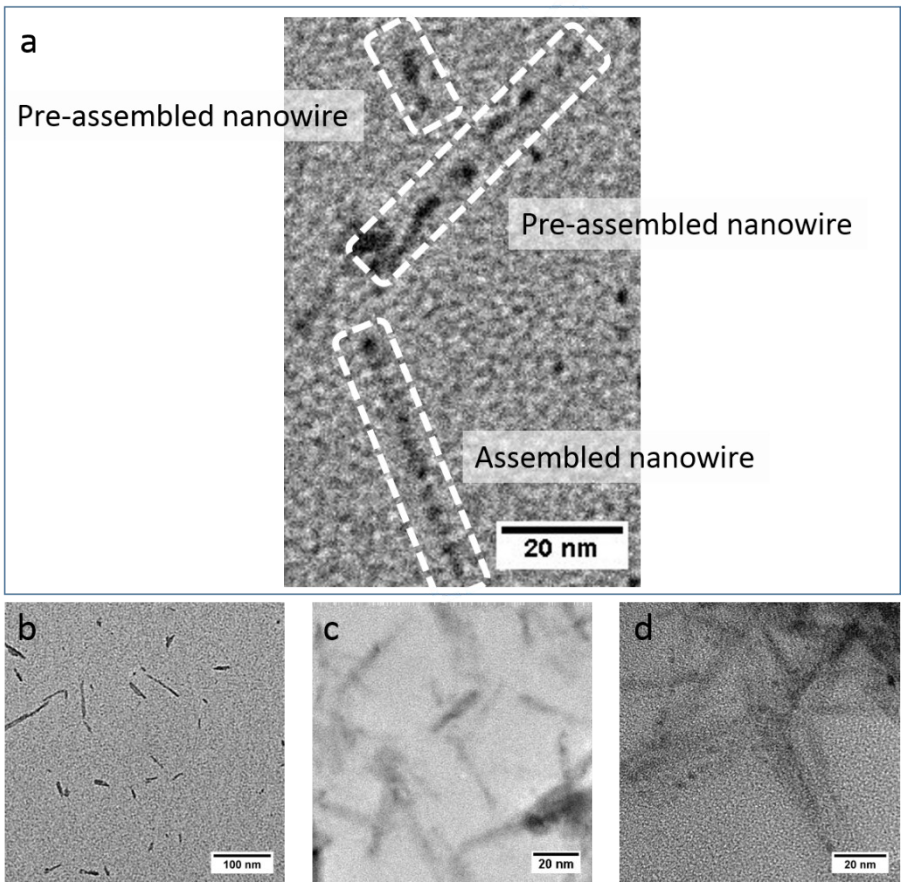

Figure S6. Selected TEM images of Cu_2O nanowires synthesized at 90℃. The dynamic electrophoretic environment causes in sample location, therefore there is a chance to observe nanowires that are occurring different assembly stages (i.e., preassembled particles, preassembled wires, and well-assembled wires.) in one TEM specimen. Preassembled nanocrystals and discontinuous/short preassembled nanowires, which is obviously assembled from nanocrystals, can be seen in above TEM images. This observation indicates that the long-range ordering nanowires form via oriented particle attachment.

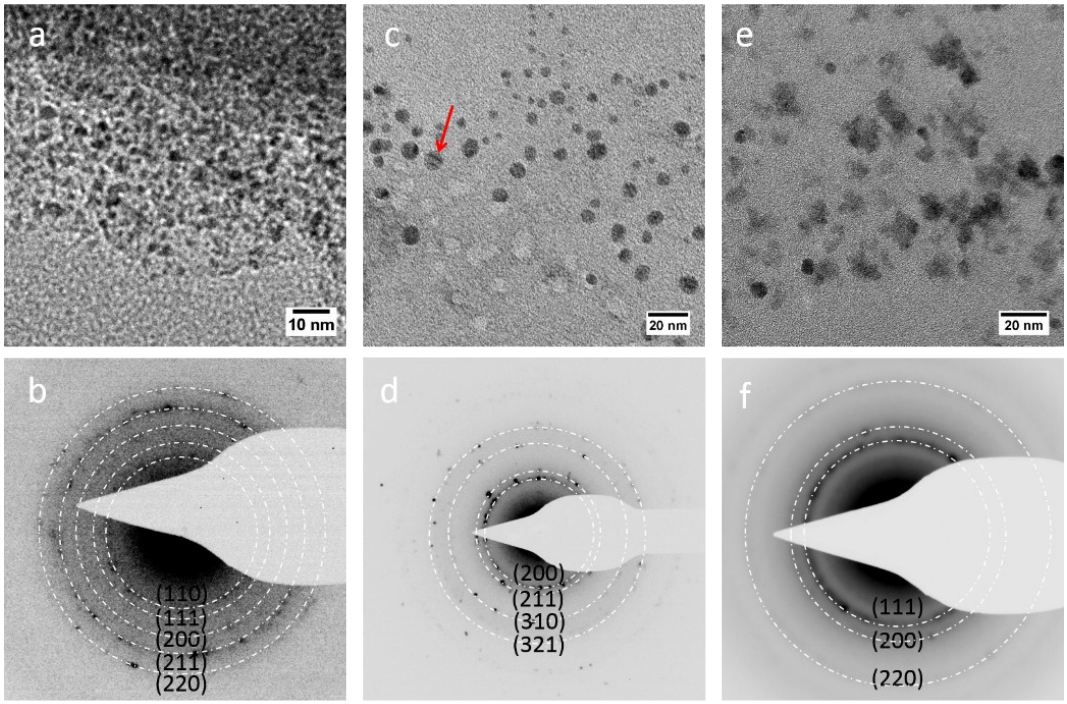

Figure S7. TEM images and corresponding SAED patterns of (a and b) QDs synthesized after ~5 min at 25℃, (c and d) coalesced QDs synthesized after ~1 min at 90℃, and (e and f) further coalesced QDs synthesized after ~5 min at 90℃. All samples are cubic Cu_2O according to SAED patterns. Atomic planes are partially indicated in the SAED patterns, while others are invisible from corresponding selected area at the applied TEM beam intensity. It is clear that the QDs synthesized at higher temperature tend to coalesce to form larger particles (Visible gain boundaries are indicated by the red arrow in Figure S7c). With longer reaction period, more QDs will coalesce (Figure S7e), orient, and grow into wire-like structures (see Figure 2d-f).

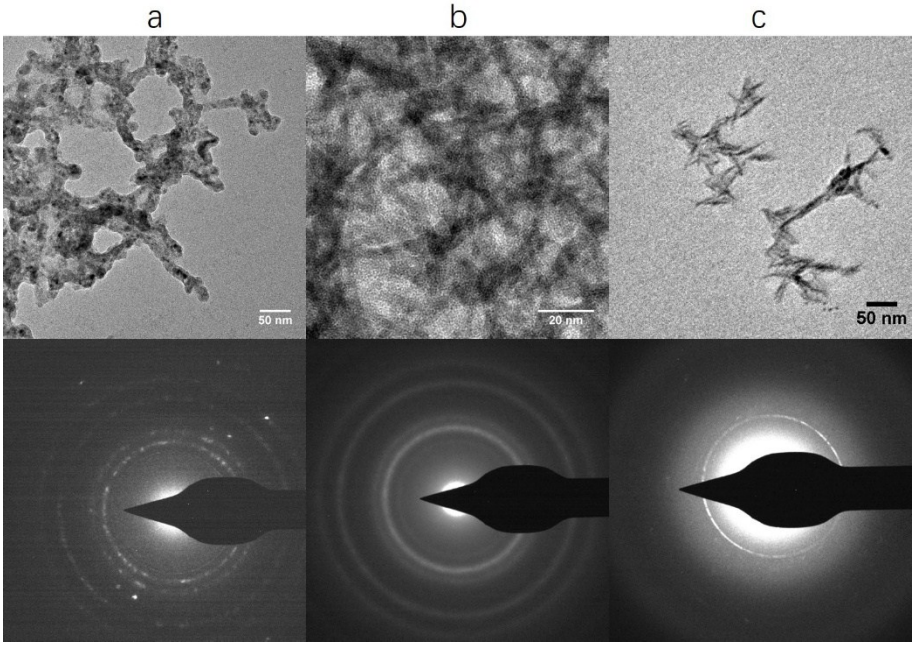

Figure S8. TEM images and the corresponding SAED patterns of (a) randomly attached Cu_2O nanoaggregation, (b) polycrystalline nanowires of Cu_2O, and (c) monocrystalline nanowires of Cu_2O. (a) and (b) show clear polycrystalline patterns. In comparison, monocrystalline nanowires of Cu_2O (c) only shows strong signal from the major plane (110), indicating the oriented attachment growth pattern of Cu_2O nanowire along the [110] direction, which is in agreement with the results reported in our manuscript. The SAED patterns deliver the crystal structure information of a considerable number of samples, declaring the statistically significance.

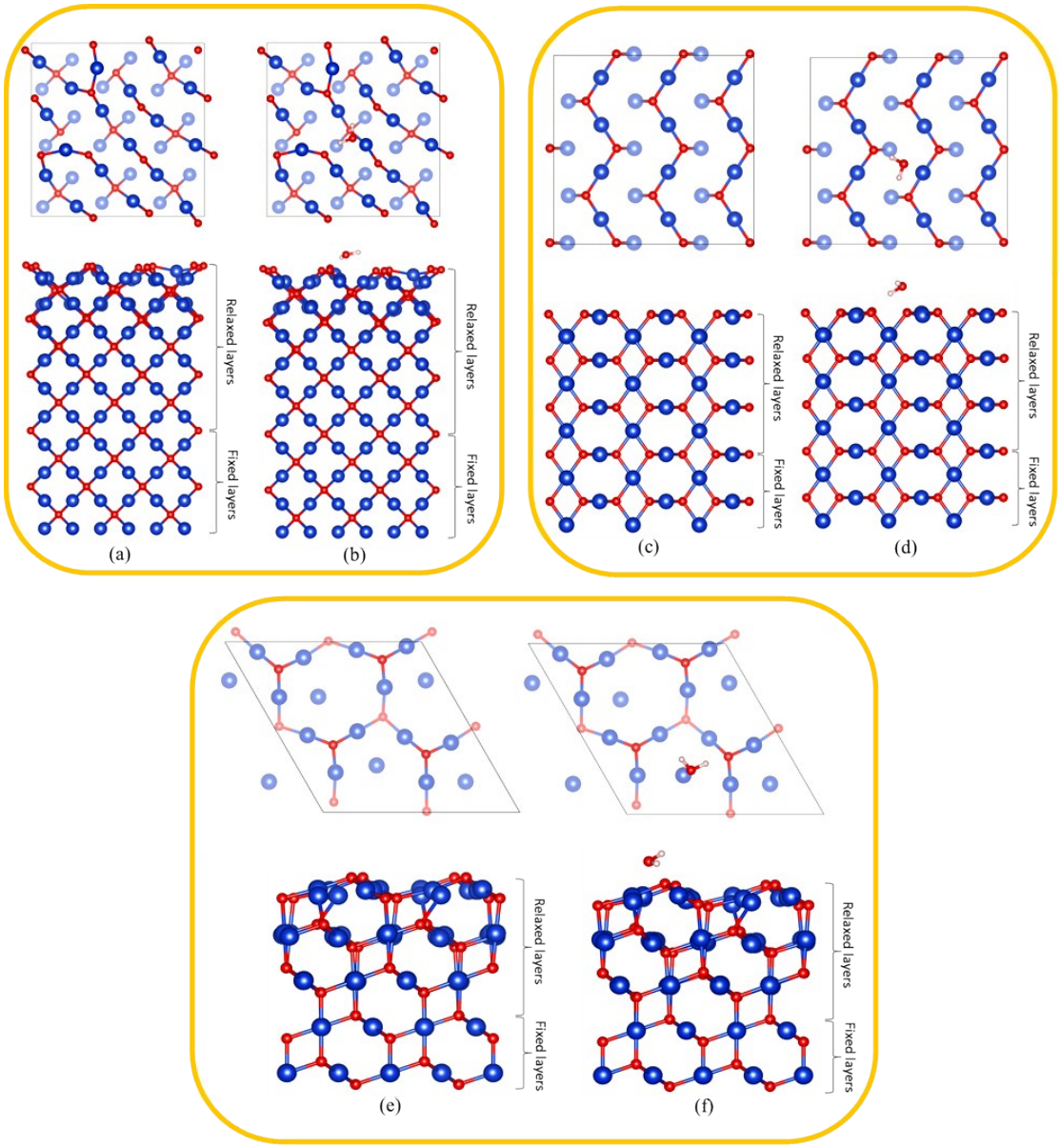

Figure S9. The configurations of (3×3) $Cu_2O(100)$:O surface, (3×2) $Cu_2O(110)$:CuO surface and (2×2) $Cu_2O(111)$:O surface and the stable configurations with water molecule adsorption. (a) Side and top view of the fully relaxed (3×3) $Cu_2O(100)$:O surface. (b) Side and top views of the configurations of the configuration with a water molecule adsorbed on the fully relaxed (3×3) $Cu_2O(100)$:O surface. (c) and (d) present the fully relaxed structure of (3×2) $Cu_2O(110)$:CuO surface and the stable configuration with a water molecule, top and side views are shown. (e) and (f) are the fully relaxed configurations of (2×2) $Cu_2O(111)$:O surface and the stable structure with a water molecule adsorbed, top and side views are shown.

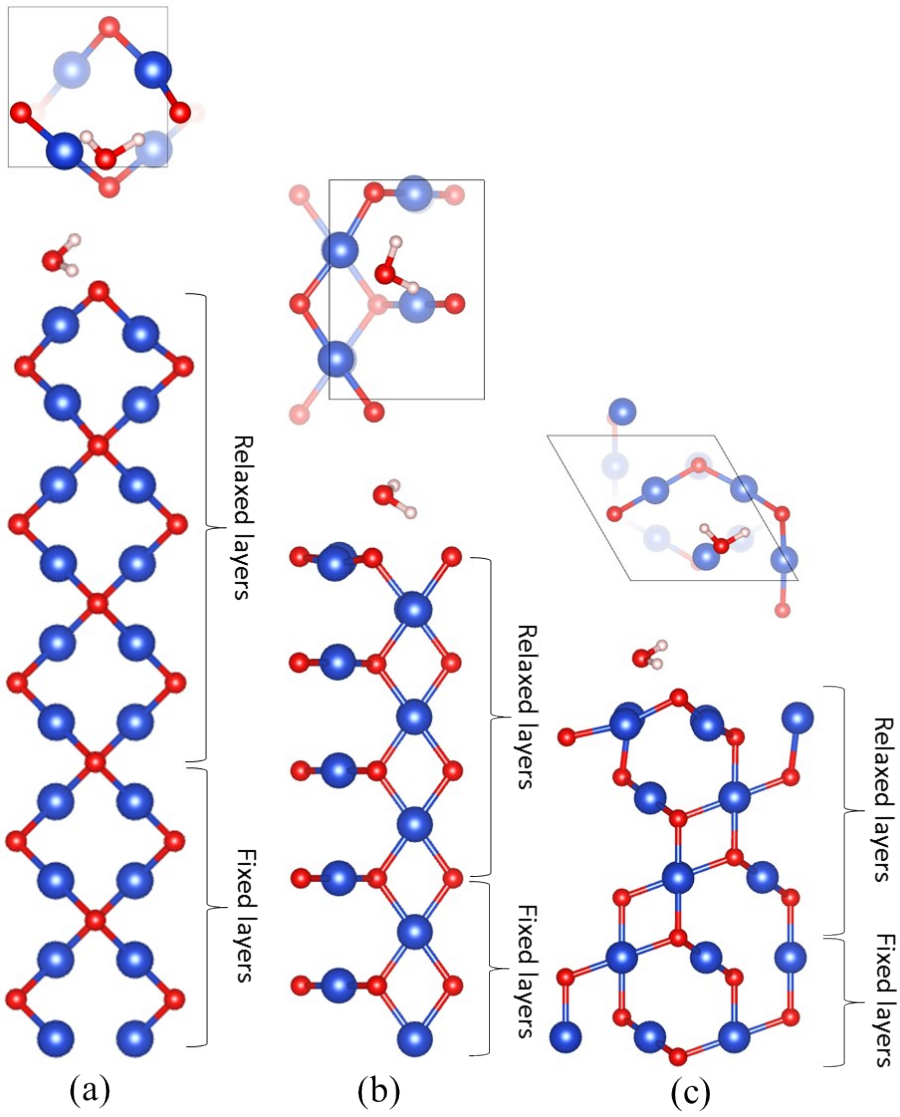

Figure S10. The stable configurations of a water molecule adsorbed on (a) (1×1) Cu_2O(100):O surface, (b) (1×1) Cu_2O(110):CuO surface and (c) (1×1) Cu_2O(111):O surface.

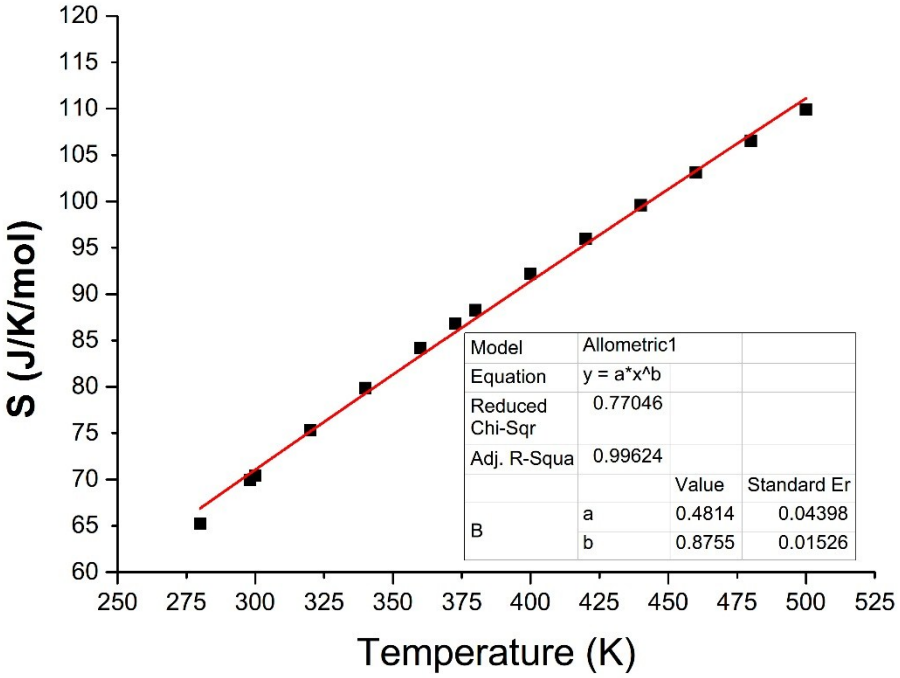

Figure S11. Fitted parameters and curves of the entropy of liquid water. The fitting data are from NIST-JANAF Thermochemical TABLEs (http://kinetics.nist.gov/janaf/).

Characterizations. We performed TEM, HRTEM, and EELS on Tecnai G2 T20 and Titan 80-300ST TEMs from FEI Company. Au grids with holey carbon support films were used as support materials for TEM imaging. XPS (Thermo Scientific) was performed to analyze the compositions of samples, with Al-Kα (1486 eV) as the excitation X-ray source. Samples were collected from the Milli-Q water solution and dried on Si substrates. The pressure of the analysis chamber was maintained at 2×10^{-10} mbar or lower during measurements.

Reference

1. C. C. Ahn, O. L. Krivanek, R. P. Burgner, M. M. Disko, P. R. Swann, EELS atlas: a reference guide of electron energy loss spectra covering all stable elements. (Gatan, Warrendale, PA, 1983)