Supporting Information

Controlling Surface Termination and Facet Orientation in Cu_2O Nanoparticles for High Photocatalytic Activity: A Combined Experimental and Density Functional Theory Study

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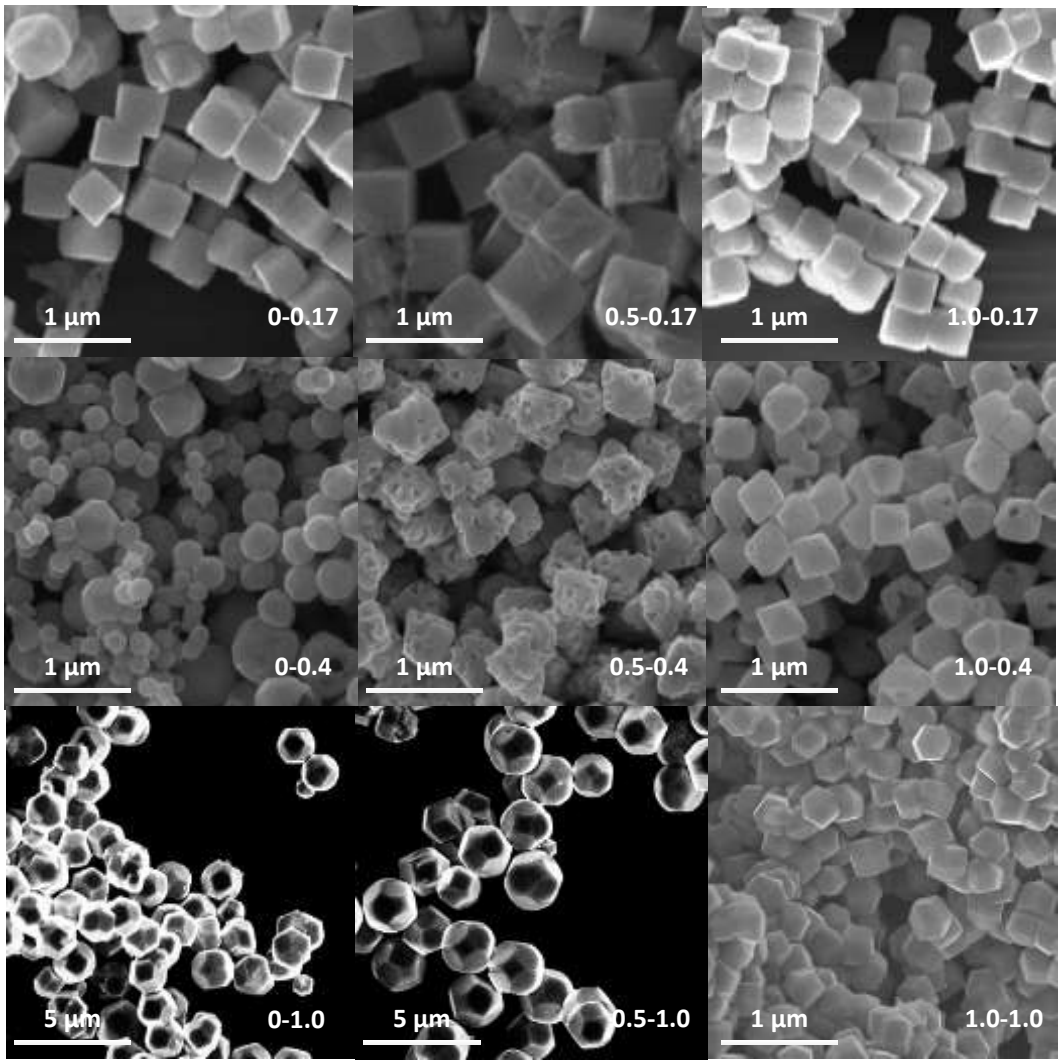

Figure S1. Low-magnification SEM images of Cu_2O nanocrystals.

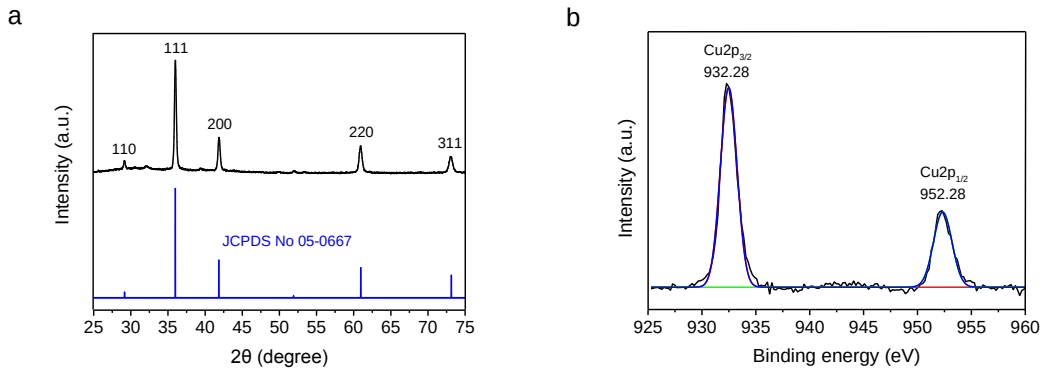

Figure S2. (a) XRD, and (b) XPS patterns of the Cu_2O nanocrystals.

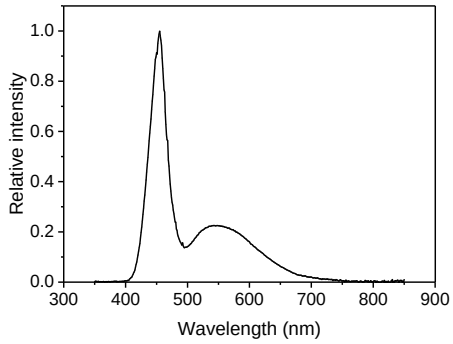

Figure S3. Spectra of visible LED light source.

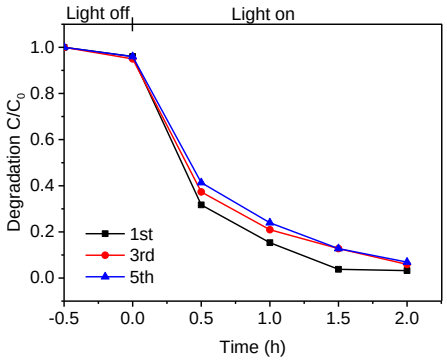

Figure S4. Cycling runs of photocatalytic reactions using sample (1.0-1.0).

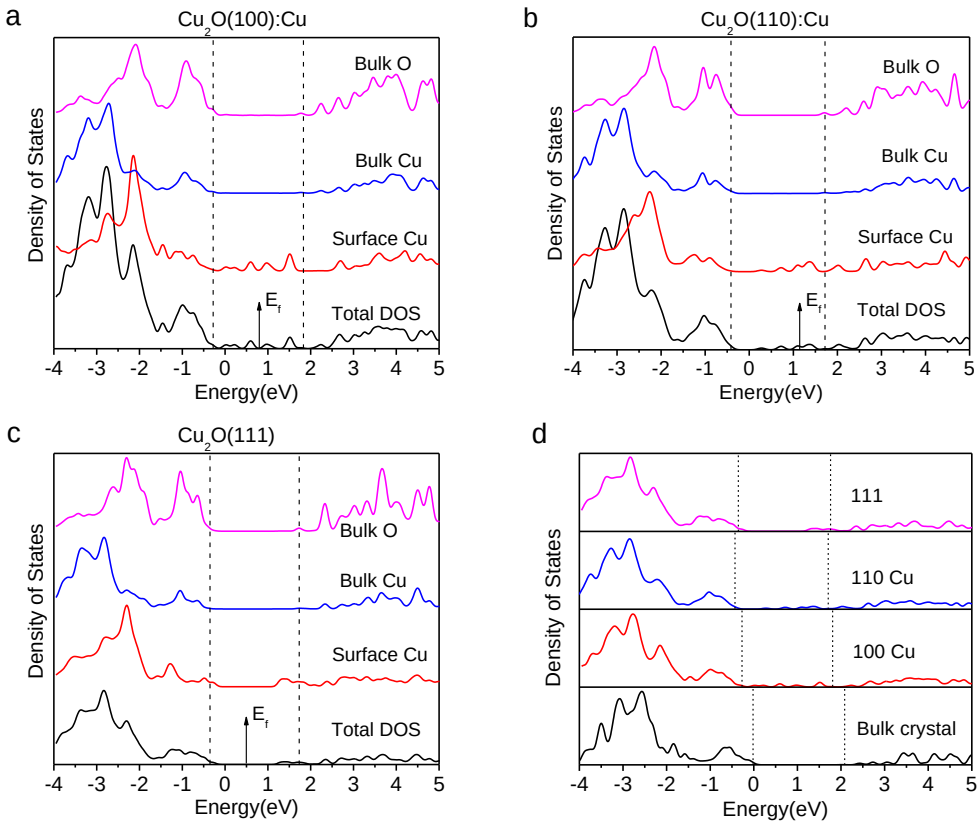

Figure S5. Partial DOS of (a) Cu_2O (100): Cu, (b) Cu_2O (110): Cu, and (c) Cu_2O (111) surfaces. (d) Band edge comparison of Cu_2O surfaces and Cu_2O bulk crystal; the bands are aligned by the 3p core level of Cu at -73 eV.

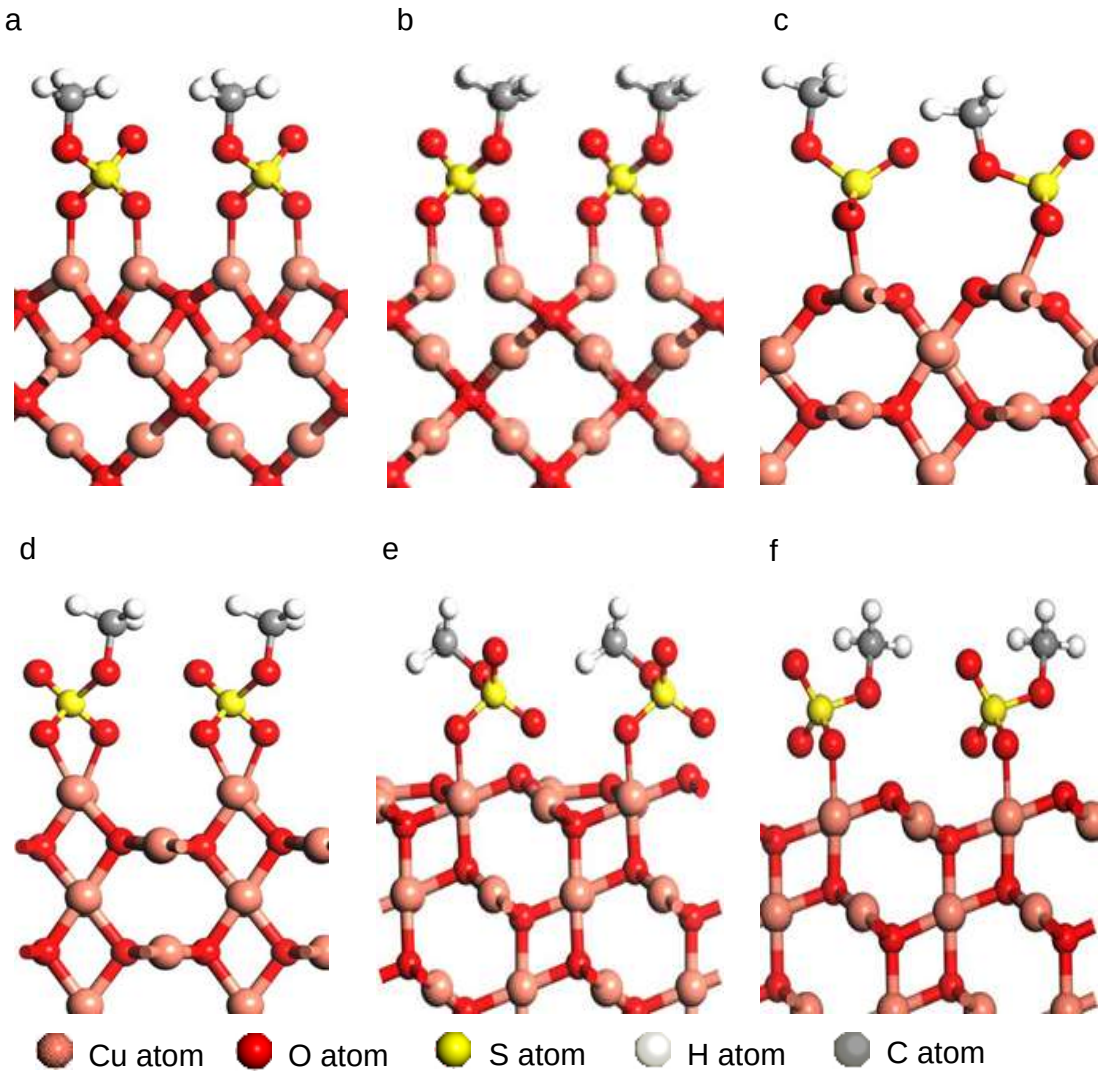

Figure S6. Atomic structures of SO_4CH_3 group adsorbed: (a) Cu_2O (100): O, (b) Cu_2O (100): Cu, (c) Cu_2O (110): O, (d) Cu_2O (110): Cu, (e) Cu_2O (111): O, and (f) Cu_2O (111) surfaces model of SDS adsorbed Cu_2O surfaces.

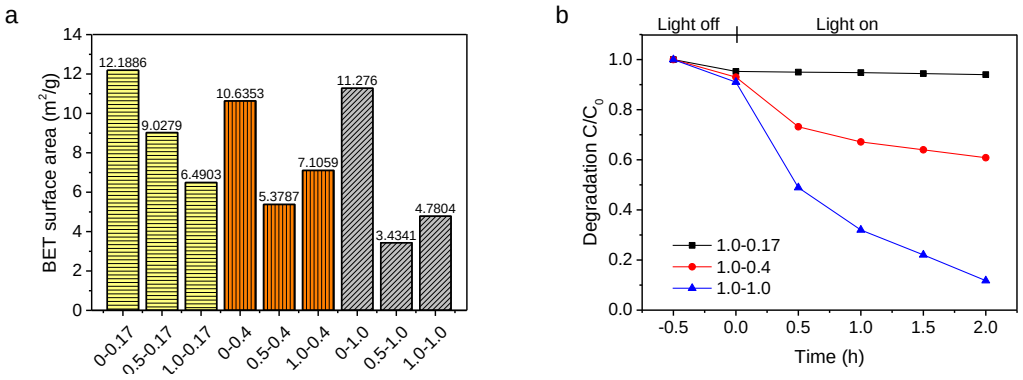

Figure S7. (a) BET surface area of all samples; (b) MO degradation using samples (1.0-0.17), (1.0-0.4) and (1.0-1.0) with a total surface area of 0.1 m^2.