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First principles investigations on the stability and catalytic reactivity of Cu2O surfaces LIANG LI, YIMIN WU, TIJANA RAJH, IAN MCNULTY, ZHONGHOU CAI, JEFF GUEST, YUZI LIU, MARIA CHAN, Argonne National Laboratory — Cu_2O is an attractive candidate as a next-generation photocatalyst for CO_2 reduction because of its high solar spectrum absorption coefficient and small electron affinity. It is observed experimentally, by Electron Paramagnetic Resonance (EPR) and Scanning x-ray fluorescence microscopy (SXFM), that the surface Cu atoms have various oxidation states, and different sites have different affinities for CO_2 and intermediate products. In this work, we employ first principles density functional theory (DFT) calculations to calculate the free energies of various low-index Cu_2O surfaces and further identify the change of surface Cu oxidation states upon the creation of surface defects and during the photocatalytic process. The reactivity of Cu_2O surfaces with various defect types and concentrations are also predicted.

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