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Scanning tunneling microscopy study of Cu2O surface facets for molecular adsorption RUI ZHANG, LIANG LI, MARIA K. CHAN, JEFFREY R. GUEST, Argonne Natl Lab — Cu ions on cuprous oxide (Cu2O) crystalline facets play important roles in the catalytic reactions, such as CO oxidation and methanol synthesis. Unfortunately, the active sites for the chemical reactions on the surface, are still unclear due to the lack of knowledge on the chemisorption and dissociation of reactant molecules on Cu2O surfaces. Studies mainly focused on defining the surface structures and adsorption of molecules have been performed by first principles density functional theory (DFT) calculations, low-energy electron diffraction (LEED), and ultrahigh-vacuum scanning tunneling microscopy (STM). However, apart from the Cu2O(100) surface, other crystalline surfaces, such as (111) and (110), which have been suggested as more chemically active for catalysis, have been scarcely investigated. Herein we discuss a combined STM-DFT study of Cu2O(111) and (110) surfaces to determine the stable structure under either oxygen-poor or oxygen-rich condition. The combined approach allows us to also determine the structure of surface defects. Active sites that are possible for dissociative adsorption on the Cu2O crystalline surface are also investigated by direct imaging of the surface adsorption with CO2 molecules and corresponding DFT calculations.

Rui Zhang
Argonne Natl Lab

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