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High Coverage Oxidation and diffusion on the Cu(001) Surface

WILLIE MADDOX, NAIL FAZLEEV, University of Texas at Arlington — The structures formed on oxidized transition metal surfaces vary from simple adlayers of chemisorbed oxygen to more complex structures which result from the diffusion of oxygen into subsurface regions. In this paper, an *ab-initio* investigation of the stability and electronic structure of the Cu(001) missing row reconstructed surface at various surface and subsurface oxygen coverages ranging from 0.5 to 1.5 monolayers is presented using density functional theory (DFT). Results of calculations regarding geometrical properties such as interatomic distances and changes in interlayer spacing as well as electronic properties including changes in adsorbate binding energy, electron work function, surface dipole moment, and deformation electron density as a function of oxygen coverage are also discussed. The studied structures are all found to be energetically more favorable as compared to structures formed by pure on-surface oxygen adsorption. We observe an increase in the work function and surface dipole moment when oxygen atoms occupy subsurface sites which can be attributed to significant charge redistribution within the first two layers, buckling effects within each layer and interlayer expansion.

Willie Maddox
University of Texas at Arlington

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