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High Coverage Oxidation of the Cu(001) Surface: A Density Functional Study¹ W.B. MADDOX, N.G. FAZLEEV, University of Texas at Arlington — The study of oxygen adsorption on transition metal surface is important for the understanding of corrosion, heterogeneous catalysis, and oxide growth. 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 sub-surface regions. In this paper, an ab-initio investigation of stability and associated physical and electronic properties of different adsorption phases of oxygen on the Cu(001) missing row reconstructed surface using density functional theory in the generalized gradient approximation, is presented. Results of calculations regarding geometrical as well as electronic properties including changes in electron work function, difference electron density and density of states as a function of oxygen coverage are also discussed. Furthermore, the chemistry of metal-adsorbate bonding is studied with primary interest being paid to high coverage oxygen adsorption.

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