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Ab-initio study of the O covered Cu(100), Cu(110), and Cu(111) surfaces W.B. MADDOX, N.G. FAZLEEV, Department of Physics, University of Texas at Arlington — The study of adsorption of oxygen on transition metal surface is important for the understanding of oxidation, heterogeneous catalysis, and metal corrosion. The structures formed on transition metal surfaces vary from simple adlayers of chemisorbed oxygen to oxygen diffusion into the sub-surface region and the formation of oxides. In this work we present an ab-initio investigation of stability and associated physical and electronic properties of different adsorption phases of oxygen on Cu(100), Cu(110) and Cu(111) as well as of the clean Cu surfaces using density functional theory in the generalized gradient approximation and a four-layer slab to model the ideal Cu surfaces. In particular, we fully optimize the geometry of the surfaces with adsorbed oxygen and study the electronic structure, the changes in electron work function, surface energy, and interlayer spacings as a function of oxygen coverage. Furthermore, we study the chemistry of the metal-adsorbate bonding. Results and analysis are also presented for the Cu20 (100) surface. We compare our results to both experimental data and other theoretical models.

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