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Density Functional Study of the Oxygen Adsorption on the Cu(110) Surface<sup>1</sup> ANTOINE OLENGA, N.G. FAZLEEV, Department of Physics, University of Texas at Arlington — Copper based catalysts are of importance to a number of industrial processes including the synthesis of methanol, the reduction and decomposition of nitrogen oxides, and treatment of waste water. In copper catalysis surface oxidation and oxidic overlayers are believed to play a crucial role. In this work using density functional theory within the generalized gradient approximation we have studied the stability and associated electronic properties of different adsorption phases of oxygen on the Cu(110) surface. Especially, we have focused on studies of changes in the interlayer spacing, electron work function, surface energy, electronic density, density of states, and band structure of the Cu(110) surface with oxygen coverage. We have examined the cases of the adsorption of oxygen at various coverages on the nonreconstructed and added row reconstructed Cu(110)surface. Calculations of electronic properties from first principles have been also performed for the (110) surface of Cu2O to use for comparison. The first-principles calculations in this work have been performed using DMOl3 code. The obtained theoretical results have been compared with available experimental data.

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