

Abstract Submitted
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Properties of the Oxidized Cu(110) Surface: The DFT study AN-TOINE OLENGA, N.G. FAZLEEV, University of Texas at Arlington — The study of adsorption of oxygen on transition metal surfaces is important for the understanding of oxidation, heterogeneous catalysis, and metal corrosion. In this work we have studied from first principles the changes of electronic properties of the Cu(110) surface due to oxygen adsorption. Especially, we have focused on studies of changes in the work function, electronic density, interlayer spacing, density of states and band structure with oxygen coverage. Calculations of electronic properties from first principles have been also performed for the (110) and surface of Cu_2O to use for comparison. The first-principles calculations in this work have been performed on the basis of the Density Functional Theory and using DMO13 code. The obtained theoretical results have been compared with available experimental data.

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