Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Electronic and Structural Properties of the Oxidized Cu(110) Surface ANTOINE OLENGA, N.G. FAZLEEV, Department of Physics, 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 present an ab-initio investigation of stability and associated physical and electronic properties of different adsorption phases of oxygen on Cu(110). Especially, we focus on studies of changes in the work function, surface energy, electronic density, interlayer spacing, density of states, and band structure of the Cu(110) surface with oxygen coverage. We examine the cases of high oxygen coverage of the reconstructed Cu(110) surface when the oxygen atoms occupy on-surface as well as sub-surfaces sites. 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 on the basis of density functional theory and using DMOl3 code. The obtained theoretical results have been compared with available experimental data. This work was supported in part by the National Science Foundation Grant DMR-0907679 and the GAANN grant P200A090284.

Nail G. Fazleev
Department of Physics, University of Texas at Arlington

Date submitted: 20 Nov 2012 Electronic form version 1.4