Abstract Submitted
for the TSS12 Meeting of
The American Physical Society

**First-Principles Study of Properties of the Oxidized Cu(110) and Cu(111) Surfaces** 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 have studied from first principles the changes of electronic properties of the Cu(110) and Cu(111) surfaces 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 (111) surfaces of Cu2O to use for comparison. The first-principles calculations in this work have been performed on the basis of the Density Functional Theory and using DMOl3 code. The obtained theoretical results have been compared with available experimental data.

Nail Fazleev
Department of Physics, University of Texas at Arlington

Date submitted: 21 Feb 2012 Electronic form version 1.4