Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

First principles studies of CO adsorption and oxidation on the $Cu_2O(100)$ surface[1] SERGEY STOLBOV, DUY LE, TALAT S. RAHMAN, Physics Department, Kansas State University — This work is motivated by the experimental results [1] indicating that the rate of CO oxidation on Cu_2O surface is much higher than that on Cu and CuO surfaces. To gain insight into the nature of this effect we study from first principles the energetics of adsorption and oxidation of CO on $Cu_2O(100)$. Applying the *ab initio* thermodynamics approach [2] to the surface in contact with gaseous O_2, we find that the O-termination of $Cu_2O(100)$ is preferred for all reasonable range of temperature and the O_2 pressure. We find that CO adsorbed on surface O associates with it to form CO_2 without any activation barrier. On the other hand, CO adsorbing on a surface Cu atom, it is found to slide first towards the neighboring O atom to form CO_2 as in the previous case. We analyze the local densities of electronic states and valence charge densities of the systems to rationalize the obtained results.

1. T.-J. Huang and D.-H. Tsai, Catal. Lett. 87, 173 (2003).

2. K. Reuter and M. Scheffler, Phys. Rev. B **65**, 035406 (2002).

[1]Work supported in part by DOE under grant No. DE-FGO3-03ER15445. Computational resources provided by NSF Cyberinfrastructure and TeraGrid, grant No: DMR050039N

Sergey Stolbov

Date submitted: 30 Nov 2005 Electronic form version 1.4