First principles studies of CO adsorption and oxidation on the Cu$_2$O(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$_2$O 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$_2$O(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$_2$O(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.


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

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Date submitted: 30 Nov 2005

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