Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Investigation of the Role of Surface Oxides in Catalysis by Gold Nanoparticles HONGQING SHI, CATHERINE STAMPFL, The University of Sydney, Sydney, Australia — In contrast to the long held view that gold is catalytically inert, it is now well known that supported gold nanoparticles are notably more active than other transition metals for low temperature catalytic oxidation of CO, as well as promoting several other catalytic reactions [1]. This has stimulated huge efforts in an attempt to understand the mechanisms responsible for the high activity, including investigations into the nature of oxygen on gold surfaces [2]. Through density-functional theory and the approach of *ab initio* thermodynamics [3] we have found that on the gold (111) surface, thin oxide-like structures are significantly more stable for the pressure and temperature conditions of CO oxidation. The energetic preference for such partially oxidized gold, is in accord with very recent experimental results [4]. For the identified lowest energy surface oxide-like structure, we investigate the adsorption of CO on the surface and determine the reaction pathways for CO oxidation.

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[3] K. Reuter, C. Stampfl and M. Scheffler, in Handbook of Materials Modeling, Volume 1, Fundamental Models and Methods, Sidney Yip (Ed) 2005, 149-194.
[4] L. Fu *et al.* J. Phys. Chem. B 109, 3704 (2005).

Hongqing Shi
The University of Sydney, Sydney, Australia

Date submitted: 19 Nov 2006 Electronic form version 1.4