

Abstract Submitted
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First-principles Investigation of the Stability of Surface Gold Oxides on Au(111) HONGQING SHI, CATHERINE STAMPFL, The University of Sydney — In contrast to the long held view that gold is catalytically inert and as such uninteresting, it is now well known that Au is significantly more active than Pt in the catalytic oxidation of CO under basic environments. Au can also promote many other reactions in the form of nanoparticles on metal oxide and activated carbon supports [1]. This has simulated 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]. In the present work we have investigated the relative stability of oxygen adsorbed on and under the Au(111) surface, as well as thin surface oxides. We identify structures in which the binding of atomic oxygen is stronger than that at under-coordinated surface Au atoms (e.g. at steps). To determine the stability of the structures for different pressure and temperature conditions, we use the approach of *ab initio* thermodynamics [3], which indicates that these structures should be stable under certain catalytic conditions.

[1] Haruta, Catal. J. New. Mater. Electro. Sys. **7**, 163 (2004).

[2] R. Meyer, *et al.*, Gold Bull. **37**, 72 (2004), and references therein.

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

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