Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Adsorption and Diffusion of Pt and Au on the Stoichiometric and Reduced TiO_2 Rutile (110) Surfaces[1]

HAKIM IDDIR, SERDAR OGUT, University of Illinois at Chicago, NIGEL BROWNING, University of California Davis and Lawrence Berkeley National Laboratory, MARK DISKO, Exxon-Mobil Research and Engineering

— A comparative first principles pseudopotential study of the adsorption and migration profiles of single Pt and Au atoms on the stoichiometric and reduced TiO_2 rutile (110)surfaces is presented. Pt and Au behave similarly with respect to (i) most favorable adsorption sites, which are found to be the hollow and substitutional sites on the stoichiometric and reduced surfaces, respectively, and (ii) the large increase in their binding energy (by $\sim$ 2 eV) when the surface is reduced. Pt, on the other hand, binds more strongly (by $\sim$ 2 eV) to both the stoichiometric and reduced surfaces. The migration profiles of the two metals also display interesting similarities and differences. In particular, although the energy barrier for both Pt and Au diffusion on the stoichiometric surface is rather low (0.1 - 0.2 eV), Pt displays a one-dimensional migration pattern, while Au migration is two-dimensional. In contrast, the energy barrier on the reduced surface is significantly higher ($\sim$ 0.5 eV) for Pt than Au. These results for Pt,Au/TiO_2 are discussed in connection with the activity of the two metals and the origin of the strong-metal-support-interaction phenomenon.

[1] Work Supported by ACS PRF Grant #s 40028-AC5M and 37552-AC5

Serdar Ogut
University of Illinois at Chicago

Date submitted: 21 Mar 2013

Electronic form version 1.4