Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Preferential Growth of Pt Particles on Rutile TiO_2[1] VLADIMIR SKAVYSH, HAKIM IDDIR, SERDAR OGUT, University of Illinois at Chicago, NIGEL BROWNING, University of California Davis and NCEM Lawrence Berkeley National Laboratory — Pt/TiO_2 is the prototype system exhibiting strong-metal-support-interaction phenomenon. The characterization of a real Pt/TiO_2 catalyst system through a combination of atomic resolution Z-contrast images and electron energy loss spectroscopy in the scanning transmission electron microscope has revelaed an unexpected result: Pt particles have a strong tendency to nucleate on the rutile phase of TiO_2 rather than anatase. In order to address the selective growth of Pt on rutile, Pt atom binding energies on stoichiometric and reduced TiO_2 surfaces and surface oxygen vacancy formation energies have been calculated using first principles density functional theory calculations for both rutile and anatase phases.

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

Serdar Ogut
University of Illinois at Chicago

Date submitted: 01 Dec 2004 Electronic form version 1.4