Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

**First principles thermodynamics studies on the surface structures of Pt-alloy catalyst as a function of the surface segregation, co-adsorption and particle size** BYUNGCHAN HAN, GERBRAND CEDER, Massachusetts Institute of Technology — Segregation in alloy catalysts can be significantly affected by the chemical environments. Using density functional theory coupled to the cluster expansion technique we study how adsorption of chemical species and bulk alloying change the surface structures and hence reactivity of Pt. We find that chemical adsorbates (O, OH, CO and water etc,) can change surface segregation energy of alloy elements dramatically in both bulk and nano-sized Pt. It implies that the interactions between adsorbates and surface atoms are important to understand the surface morphology and catalyst activities. We also find that Pt oxide (Pt-O or Pt-OH) has a higher reactivity to CO oxidation than pure Pt. On the other hands, Ru alloying on the Pt surface without adsorbates enhances the CO adsorption on Pt. We also investigate the effect of nanoparticle size of the on surface segregation and CO oxidation.

Byungchan Han
Massachusetts Institute of Technology

Date submitted: 04 Dec 2005 Electronic form version 1.4