Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Atomistic simulations of surface segregation in bimetallic Pt-M catalyst nanoparticles (M=Ni, Re, Mo) GUOFENG WANG, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, M.A. VAN HOVE, Lawrence Berkeley National Laboratory, Berkeley, CA 94720; Dept. of Physics, University of California, Davis, CA 95616, P.N. ROSS, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, M.I. BASKES, Los Alamos National Laboratory, Los Alamos, NM 87545 —
To design Pt bimetallic catalyst nanoparticles for their applications in fuel cells, we have developed interatomic potentials within the modified embedded atom method for Pt-Ni, Pt-Re, and Pt-Mo alloy systems. These potentials were used in an investigation of the segregation of Pt atoms to the surfaces of nanoparticles with sizes from 2.5 nm to 5 nm. We draw the following conclusions from our Monte Carlo simulations at T= 600 K. Due to surface segregation, (1) Pt-Ni nanoparticles form a surface-sandwich structure in which the Pt atoms are strongly enriched in the outermost and third layers while the Ni atoms are enriched in the second layer; (2) the equilibrium Pt-Re nanoparticles adopt a core-shell structure, with a highly Pt-enriched shell surrounding a Pt-Re core; and (3) Pt slightly segregates to the surface of Pt-Mo nanoparticles and preferentially occupies the facet sites in the surfaces. This work was supported by the U.S. Department of Energy under Contract No. DE-AC03-76SF00098 at LBNL and W-7405-ENG-36 at LANL.

Guofeng Wang
Lawrence Berkeley National Laboratory

Date submitted: 30 Nov 2004 Electronic form version 1.4