Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Single oxide overlayers grown on top of another oxide: Their stability, interaction with metal nanoparticles, and contribution to catalytic activity SERGEY RASHKEEV, Idaho National Laboratory — Oxides are widely used as catalysts as well as supports for catalytically active metal nanoparticles. The catalytic activity of the system depends on many different factors such as anchoring, sintering, decomposition, and diffusion of metal atoms/clusters on the oxide surface. Here we use a combination of first-principles density-functional calculations and molecular dynamics simulations to investigate how all of these factors may change when the surface of the oxide support is modified by an additional single overlayer of another oxide positioned on it. In particular, we found that deposited monolayer oxide films may show instabilities that result in formation of strong anchoring sites for metal atoms/clusters. Also, an atomic-scale roughness introduced in such a way may slow down the surface diffusion processes and inhibit nanocluster growth/sintering. For example, a single layer of SiO2 on a TiO2 substrate may significantly increase the stability of Au nanoparticles and the efficiency of the catalytic CO oxidation. The author thanks Dr. Steven Overbury (Oak Ridge National Laboratory) for attracting his attention to this problem and INL Laboratory Directed Research and Development program and the U. S. Department of Energy, Office of Nuclear Energy under DOE Idaho Operations Office Contract DE-AC07-051D14517 for financial support.

Sergey Rashkeev
Idaho National Laboratory

Date submitted: 27 Nov 2007 Electronic form version 1.4