Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Adsorptive and chemical properties of supported silver clusters SARA E. MASON, ELIZABETH A. SOKOL, University of Pennsylvania, VALENTINO R. COOPER, Rutgers, The State Univ. of N.J., ANDREW M. RAPPE, University of Pennsylvania — Unlike bulk metal slabs, clusters of transition metals on nonmetallic supports have a finite electron reservoir. Additionally, the interaction of clusters with the support can lead to polarization in the cluster. These effects give rise to adsorption properties quite different from those of bulk metal. We characterize the adsorption of different atomic and molecular species on silver clusters supported by Al-terminated alpha-alumina using DFT/GGA calculations. A range of cluster sizes and cluster geometries is onsidered and the adsorption energetics and geometries are compared with those of bulk silver metal.

Sara E. Mason
University of Pennsylvania

Date submitted: 04 Dec 2005 Electronic form version 1.4