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Geometry and Electronic Structure of Alumina Supported Ag Clusters ELIZABETH A. SOKOL, SARA E. MASON, University of Pennsylvania, VALENTINO R. COOPER, Rutgers, The State Univ. of N.J., ANDREW M. RAPPE, University of Pennsylvania — We use DFT/GGA to model silver clusters supported on Al-terminated alpha-alumina. A variety of cluster sizes and geometry are considered. We find that the adsorption of the Ag clusters causes dramatic surface relaxations and polarization of the Ag clusters as some Ag atoms of the clusters bond with O, while others bond with Al. For comparison, we also model adsorption of a single Ag atom, which bonds at a hollow site (relative to surface oxygen). We use the electronic structure of the adsorbed clusters to interpret the bonding interaction between the Ag atoms and surface O and Al atoms. The differences in Ag-surface bonds within the cluster give rise to different electronic environments at each Ag atoms. This effect has implications of this result to reactivity.

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