Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Electronic Structure of Thiolate Covered Gold Nanoparticles[1]

YAN LI, GIULIA GALLI, FRANCOIS GYGI, University of California, Davis — We present ab initio calculations of the structural, electronic, and bonding properties of thiolate-covered gold nanoparticles that have been crystallized in recent experiments ($Au_{102}(MBA)_{44}$)[1]. We simulated exactly the same system as investigated experimentally (1596 atoms) and the results of our structural optimization confirm the stability of the experimentally determined structure. We find that the crystallized solid is a semiconductor with a sizable energy gap ($\sim$0.5 eV, within DFT), and electronic states at the valence band maximum and conduction band minimum are extended over the gold nanoparticle core and the interface. This energy gap appears to be insensitive to the type of adsorbate. We find a tendency of the adsorbate to exert "pull-out" forces on the surface gold atoms, and our analysis of chemical bonding supports the hypothesis that gold s electrons are donated to the MBA radicals so as to form a highly stable 58-electron, filled electronic shell structure. Finally, comparisons between adsorption energies in the case of gold nanoparticles and flat surfaces show that a finite curvature of the interface enhances the stability of Au-S bonds.
[1]Yan Li, Giulia Galli and Francois Gygi, ACS Nano, 2, 1896(2008)

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[1] This work was funded by NSF Grant No. DMR-0213618, No. 0749217 and by DOE/BES Grant No. DE-FG02-06ER46262.

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Date submitted: 07 Dec 2008 Electronic form version 1.4