Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Structural and electronic properties of crystals of thiolate-capped Au nanoparticles doped with donor and acceptor molecules: first-principles calculations[1] RONALDO BATISTA, Universidade Federal de Ouro Preto, JONATHAN MARTINS, HÉLIO CHACHAM, Universidade Federal de Minas Gerais — Structural and electronic properties of crystals of etiolate- capped Au nanoparticles doped with donor and acceptor molecules: first-principles calculations We perform first-principles calculations for crystals composed of periodic assemblies of Au_{38} nanoparticles that are capped with methylthiol molecules. We consider fcc structures, consistent with recent experimental results [1]. We also consider that the nanoparticle crystals can be doped with either donor (tetrabutylammonium) or acceptor (hexafluorophosphate) molecules, also consistent with recent experiments [2]. We find that the most stable positions of the dopant molecules are located near the nanoparticle surfaces, and not near interstitial positions. We also find that the electron chemical potential changes linearly with the impurity concentration, up to a critical concentration, consistent with recent experiments [2]. Above that critical concentration, a new regime is observed due to a partial charge transfer between dopants and nanoparticles. These features are reproduced by a simple capacitive model for the crystal. [1] Abécassis et al. Phys. Rev. Lett. 100, 115504 (2008) [2] Boettcher S. W. et al. Nature Mater. 6, 592596 (2007).

[1]CNPq, Fapemig and Instituto do Milnio de Nanocincias

Ronaldo Batista
Universidade Federal de Ouro Preto

Date submitted: 19 Dec 2008 Electronic form version 1.4