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Doped assemblies of Au nanoparticles: structural and electronic properties

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Assemblies of ligand-stabilized metal nanoparticles can present peculiar properties that differ from those of bulk materials The large interstitial voids in these assemblies allow them to be permeated by dopant molecules in a reversible and controllable way, inside electrochemical cells [1]. This latter property has been recently used to produce a tunable Schottky barrier between a Au nanoparticle film and a semiconductor surface [1]. Such a chemically tunable electronic device is an example of the technological potential of this new class of nanostructured materials.

In this work, we apply first-principles methods to study the changes in the properties of a periodic assembly of Au nanoparticles due to the addition of (donor) tetrabutylammonium $(C_4H_9)_4N$ molecules , or (acceptor) hexafluorophosphate (PF_6) molecules (see Fig.1). These are the molecular dopants used in recent experiments [1]. To our knowledge, this is the first *ab initio* investigation for this new type of material. We find that the most stable dopant positions are near the nanoparticle surfaces, away from the center of interstitial positions. The dopants provide an effective screening mechanism, strongly reducing the nanoparticles´ charging energies. We find a linear dependence of the Fermi level with dopant concentration, consistent with recent experiments, up to a critical concentration. For larger concentrations, a new regime is predicted. These features are well reproduced by a simple, analytical model for the material.

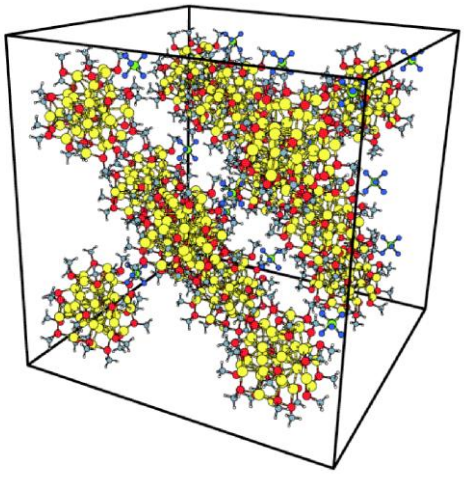

Figure 1: Periodic assembly of ligand-stabilized Au nanoparticles, doped with PF_6

Reference

[1] S. W. Boettcher et al, Nature Mat. **6**, 592 (2007).