MAGNETISM IN GOLD NANOPARTICLES AND GOLD CLUSTERS: THE ROLE OF CHEMISORPTION AND SIZE

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Abstract

The understanding of the onset of magnetism in gold nanoparticles is of practical and theoretical importance. Bulk gold is diamagnetic but nanogold displays a rather complex magnetic behavior that is both size and shape-dependent. On the practical side, there is considerable interest in different therapies based on the use of gold nanoparticles where both magnetic and optical properties can be of importance in, for example, cancer treatment.

We present quantum mechanical calculations of the electronic structure and the magnetic properties of both bare and ligand-capped gold clusters. Our results indicate that the nature of the ligand, size and shape may strongly modify the magnetic behavior of nanogold. We also found, as size increases, the emergence of a core-shell structure, where the magnetism is essentially associated to the surface atoms whereas the core is diamagnetic. Both results are of importance in interpreting recent experimental work.

We also present a mean-field, semi-classical model, that takes into account the magnetic core-shell structure of gold nanoparticles, which we found in the quantum description, and incorporates it into a statistical model. The main result that emerges from this modeling is that the magnetic moment increases up to a maximum and then decreases as a function of size, a result that has also been observed experimentally.