Permanent magnetism, in Gold nanoparticles and nanorods

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Gold nanostructures have attracted widespread attention due to their novel optical, electronic and biocompatible properties. They also exhibit a number of remarkable magnetic properties, in sharp contrast with the diamagnetic behaviour characteristic of the bulk material. In particular, thiol capped nanoparticles, 1.5 nm size, have been shown to exhibit ferromagnetic like behaviour. XMCD studies indicate that Au atoms are the magnetic moment carriers.

Using first principle calculations, we consider the bond between thiolate and small Au clusters. Surprisingly, gold thiolate exhibits a dramatic and non-intuitive distribution of charge and spin moment. Our results show that the S-Au bond is such that sulfur does not get charge and an electron is transferred to the sp states of the Au cluster. These sp electrons are almost free in the second gold layer and could orbit and it is these that are responsible for the magnetism.

It is shown that at 0K the sp surface free electrons of Au nanoparticles are distributed within an energy spectrum that may hold a giant orbital magnetic moment. The quantum number that defines the eigenstate is the orbital momentum. When the eigenstate corresponding to the Fermi level is not completely filled the residual orbital moment is of the order of the number of electrons in the band.