Electron and Spin Transport in Mn_{12} Single Molecule Magnets Bridging Gold Electrodes: How to Determine the Easy Axis Orientation Experimentally.

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Abstract

Single molecule magnets hold the promise of being the smallest possible electronic and spintronic devices. However, to realize their potential, it is necessary to contact them with electrodes and probe their transport properties by investigating how they transmit currents of spin and charge.

In this talk, I will present our tight-binding theory of Mn_{12} single molecule magnets contacted with gold electrodes. The model includes both the spatial and spin aspects of the electronic states. Spin-orbit coupling is included explicitly in the Hamiltonian and magnetic anisotropy values in agreement with experiment are obtained. I will demonstrate that Mn_{12} single molecule magnets strongly coupled to gold electrodes should exhibit strong spin filtering under appropriate conditions.

In experiments, the orientation of the molecule's easy axis relative to leads is not controllable and it has not been feasible to measure it. Our calculations reveal the possibility of determining the easy axis orientation experimentally by means of current measurements: In the molecular junction with the easy axis parallel to leads the current is predicted to be at least two orders of magnitude larger than if the easy axis is perpendicular to the leads, for molecules thiol bonded to the leads with similar gold-sulfur distances in the two cases.

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