

Abstract Submitted
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Electron and Spin Transport in Mn₁₂ Single Molecule Magnets Bridging Gold Electrodes: How to Determine the Easy Axis Orientation Experimentally¹ FATEMEH ROSTAMZADEH RENANI, GEORGE KIRCZENOW, Simon Fraser University, Burnaby, Canada — We present a tight-binding theory of Mn₁₂ single molecule magnets thiol-bonded to 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. We demonstrate that Mn₁₂ 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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