

Single Molecule Magnets: some prospects, some challenges
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Abstract

In this talk I will outline some of the promising properties of single molecule magnets (SMM), or magnetic molecules, and the challenges in their feasibilities as quantum computers (QC's). SMM's consist of monodisperse nanoscale clusters of 2 to 15, and possibly more magnetic core ions embedded in non-magnetic ligand groups, all of which pack into large, single crystalline arrays. The magnetic core ions interact mainly through Heisenberg exchange interactions. The intramolecular magnetic interaction strengths are in the range 1-100K, whereas the much weaker intermolecular magnetic interactions are about 10 mK in strength. Although antiferromagnetic (AFM) SMM's appear to exhibit more interesting low temperature quantum effects than do ferromagnetic (FM) SMM's, the latter have attracted a considerable interest, due to the suggestion that their properties might be exploited to construct useful magnetic storage devices and QC's. Two strong advantages of SMM's over other potential QC devices is that the nanoscale size of the individual molecules allows one to pack approximately 10^{20} of them in a cm^3 , and their spatial configurations are fixed. However, serious problems arise in reading and writing the information on the scale of 1 nm, and additional decoherence problems also appear to be severe.

The two SMM's studied most extensively experimentally, Fe₈ and Mn₁₂, have multiple spin-spin interactions with both AF and AFM signs and various local spin anisotropy effects within an SMM unit, and are hence difficult to model theoretically. A number of SMM's with magnetic cores consisting of just 2-4 magnetic ions have also been prepared. In these molecules the 3d-atoms link to each other through oxygen atoms giving rise to a M-O-M superexchange interaction (M=3d-atom) whose characteristics depend on the M-O-M angle. The ligands forming these links provide an opportunity for manipulating the nature and/or the strength of the exchange interaction. The magnetic interaction between the SMM's is mostly dipolar. And although it is in comparison weak, it may cause decoherence in the behavior in the presence of an external magnetic field. On the other hand, the magnetic anisotropy (caused mostly by the spin-orbital interaction in 3d-atoms placed in non-symmetric environment) determines the magnetic hysteresis. I will present some preliminary results of first principle calculations of the ferromagnetic and antiferromagnetic states of Fe₂O₂H₂ which show that the general features of the spin- and valence charge densities, and local spin resolved densities of electronic states depend strongly on the O-Fe-O angle (80° - 120°) and in are in qualitative agreement with experimental results. We have also performed calculations of the effect of the magnetic dipole-dipole interaction between SMM on the magnetization of the system at various temperatures and magnetic field to find that the dipole-dipole interaction leads to a small anisotropy which results in an additional hysteresis in M(B).