Summary of PTDC102284

Single molecule magnets (SMM) consist in clusters of metal ions with unpaired electrons, surrounded and bridged by organic ligands. The metal ions interact strongly intramolecularly and very weakly intermolecularly so that each molecule can be considered independent. The identical molecules are assembled in a periodic three-dimensional lattice. They possess a high spin ground state and strong Ising type magnetic anisotropy so that the magnetisation can be retained after the removal of the magnetic field. At very low temperatures the magnetization can be retained for several months.

SMMs are of major interest for two main reasons: their applications and the fundamental physics involved.

SMMs can be applied in the storage of information with each molecule stocking one bit of information. In a suitable disk support, these molecules can be nanoscale magnetic particles of a sharply defined size and increase the current storage capacity by 10 000. SMMs are also strong candidates for the construction of quantum computers. They offer two main advantages when compared with other candidate systems for quantum computation: chemical synthesis provides a large number of identical nano-objects in a cheap straightforward way and molecules/clusters being larger than single ion impurities relax constraints for a local read out.
The SMMs magnetic properties (ferro-, ferri-, antiferro-) can be tuned by changing the nature of the interacting metal ions, by changing the bridging ligands and by modifying the environment created by the supramolecular arrangement of the building blocks. But contrasting with their inorganic counterparts, SMMs can go beyond magnetic properties, they can be polyfunctional. Additional properties can be introduced in different ways: (i) the ligand can be the centre of this phenomenon when bearing a specific property, for example, optical in the case of an optically active ligand, magnetic when the ligand is a free radical, (ii) one of the building blocks can possess a specific property like chirality or fluorescent activity, (iii) when the materials comprise two sub-lattices (hybrid materials), one of them can bring out the magnetic properties while the other one introduce a different property.

Concerning fundamental physics, molecular magnets have actually shown, since the beginning of the 90s, captivating quantum phenomena, such as the tunnelling of magnetization through an anisotropy barrier and quantum interference (Berry's phase).
In these magnets the observed hysteresis is not due to reorientation of domains, as in conventional ferromagnets, but reflects the magnetization tunnelling between quantum states of different m, $-S<m<S$, of the total spin S of the molecule, as the external magnetic field realigns the degeneracies of different states. This process can only be observed because the relaxation time is very large compared to the measurement time. The relaxation of the magnetization becomes indeed very slow at low temperatures (of the order of several months at 2 K).

The aim of this project is to obtain new SMMs with larger metal-metal interactions so that the critical temperature would be higher and the blocking temperatures, i.e., temperatures below which the magnetization remains for several months, would also be higher.
For that a new strategy has been devised, consisting in 1) use of silicon carboxylate ligands, 2) use of different ligands with nitrogen atoms as the coordinating metal atoms, 3) build clusters of higher dimensionality based on trimers of magnetic ions bridged by aminoacids.
A theoretical study will accompany the experimental work (synthesis, structural characterization, magnetic evaluation etc) so that magneto-structural correlations can be established.