Magnetic anisotropy in mono- and bi-nuclear complexes: theoretical insight and prospects

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Abstract: Magnetic anisotropy is the origin of the single molecule magnet (SMM) behavior which is manifested by a slow relaxation of the magnetization and a blocking of the magnetization for low enough temperatures. Since this bistable behavior may lead to possible technological applications in the domain of data storage and quantum computing, the understanding of the microscopic origin of magnetic anisotropy has received a considerable interest during the last two decades.

A first study will be devoted to the rationalization of the magnitude and nature of single ion anisotropy from correlated relativistic calculations. Various strategies that have been explored in order to control the nature and tune the magnitude of the magnetic anisotropy will be presented and magneto-structural correlations will be performed.[1,2,3]

The overall magnetic anisotropy of a poly-nuclear complex comes from both the local anisotropies of paramagnetic ions and their interactions. In a first place, we will question the validity of the usual models. Then we will focus on the understanding of synergistic effects between local anisotropies in bi-nuclear complexes. [4,5,6]

Finally, some perspectives concerning both the theoretical treatment of anisotropic systems and their possible use in technological devices will be discussed.[7]

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