ZERNIKE INSTITUTE COLLOQUIUM

Thursday, December 12th, 2013

16:00h, Lecture Hall: 5111.0080 **Coffee and cakes from 15:30h**

Theoretical study of magnetic anisotropy in mono- and bi-nuclear complexes

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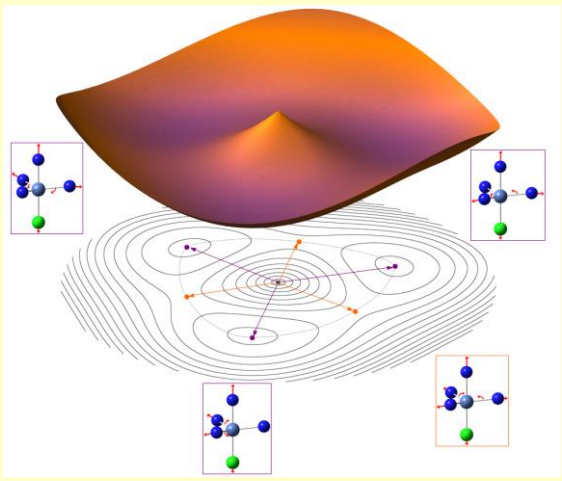
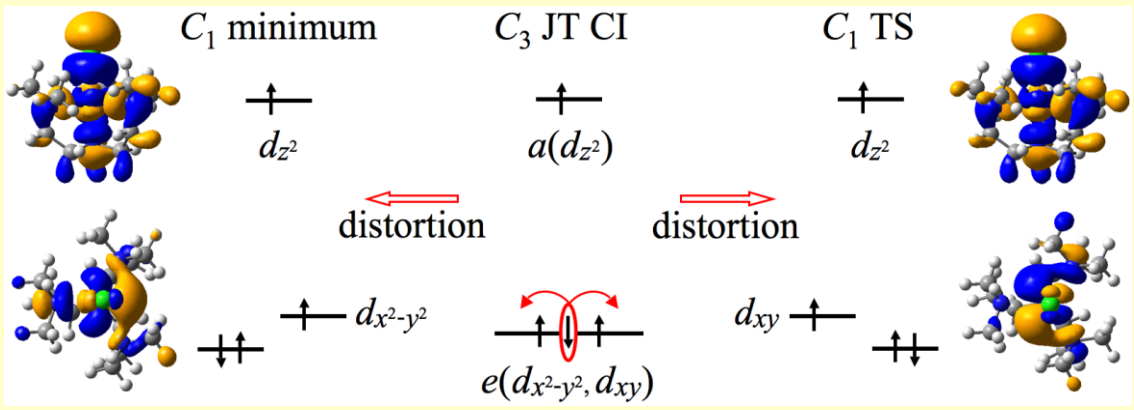
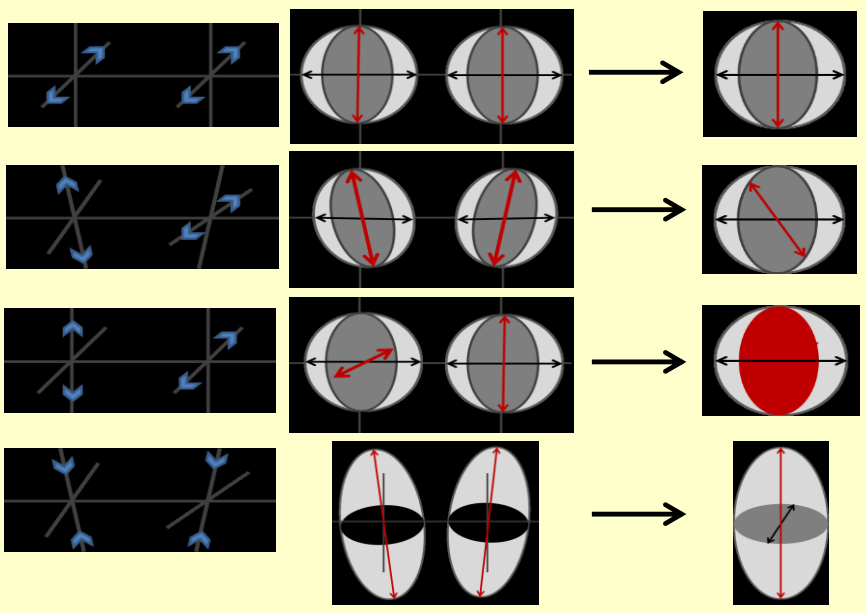
Magnetic anisotropy is the origin of the single molecule magnet (SMM) behavior which consists in a slow relaxation of the magnetization, and to a blocking of the magnetization for low enough temperatures. Since this bistable behavior may lead to possible technological applications in the domain of data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



Mono-nuclear complexes having exotic coordination of the metal ion have recently been shown to exhibit a very large magnetic anisotropy. A first study will be devoted to the rationalization of the magnitude and nature of single ion anisotropy from theoretical calculations.





The overall magnetic anisotropy of a poly-nuclear complex comes from both the local anisotropies of paramagnetic ions and their interactions. The second part of this presentation will focus on the understanding of synergistic effects between local anisotropies in bi-nuclear species for which we have both tuned the local anisotropies by imposing specific geometries and combined various types of local anisotropies .

This study follows previous works in which the method used here was successfully confronted to experimental values in series of mono- and bi-nuclear complexes.

R. Maurice et al. *J. of Chem. Theo. Comp*., **2009** 5, 11 2977; *J Chem. Theor. Chem* **2010** 6 1, 55; *J. Chem. Theor. Chem.* **2010** 6 10, 3092; *Phys. Rev. B*, **2010** 81 21, 214427; *J. Chem. Phys.* **2010** 133, 084307; *Inorg. Chem.* **2011** 50 13, 6229; Pradipto, Abdul-Muizz *et al. Phys. Rev. B* **2012**, 85, 014409; R. Maurice *et al. Phys. Rev. B* **2012**, 86, 024411; R. Ruamps et al.Chem. Euro. J. **2013**, 19, 950; R. Ruamps et al. *J. Am. Chem. Soc*. **2013**, 135, 3017A, R. Maurice *et al. Phys. Chem. Chem. Phys.*, **2013**, 15 (43), 18784.

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