

Modulation of Single-Molecule Magnet Properties: a Theoretical Investigation

Vincent Montigaud^a, Frédéric Gendron^a, Olivier Cador^a, Fabrice Pointillart^a, Boris Le Guennic^a

^aUniv Rennes, ENSCR, INSA Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) UMR 6226, F-35000 Rennes, France
vincent.montigaud@univ-rennes1.fr

In the beginning of the century, the emergence of lanthanide-based systems exhibiting slow relaxation of their magnetization opened a new chapter in the field of molecular magnetism.[1,2] These so called lanthanide-based Single-Molecule Magnets (SMMs) found many potential applications such as high-density data storage, spintronic or quantum computing.[3] On the computational point of view, the multiconfigurational wavefunction-based SA-CASSCF/RASSI-SO approach is known as a powerful tool to obtain a good description of both the electronic and magnetic features of lanthanide-based SMMs.[4] In this work, we will focus on the application of such computational protocol to describe the modulation of the SMM properties observed in two different recently characterized architectures. We will investigate the evolution of the relaxation mechanisms occurring in both an Er(III)-based polyoxometallate and an extended-tetrathiafulvalene Dy(III)-based dimer (see Figure) upon hydration/dehydration and reversible redox- and hydro-magnetic switching processes, respectively.

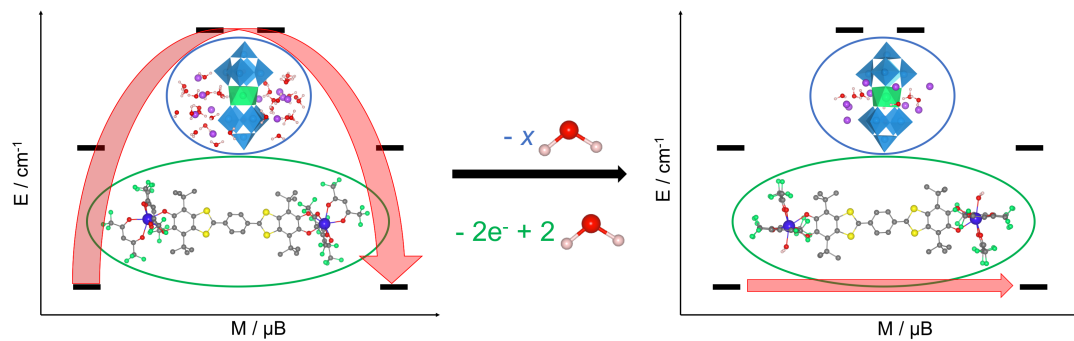


Figure: From slow (left) to fast (right) relaxation of the magnetization in the Er(III) (blue) and Dy(III) (green) systems.

References

1. N. Ishikawa, M. Sugita, T. Ishikawa, S.-Y. Koshihara, Y. Kaizu, *J. Am. Chem. Soc.* **125** (2003), 8694.
2. D. N. Woodruff, R. E. P. Winpenny, R. A. Layfield, *Chem. Rev.* **113** (2013), 5110.
3. A. Cornia, O. Seneor, *Nat. Mater.* **16** (2017), 505.
4. F.-S. Guo, B. M. Day, Y.-C. Chen, M.-L. Tong, *Science* **362** (2018), 1400.

This laboratory is part of a project that has received funding from the European Research Council (ERC) under the European Unions Horizon 2020 research and innovation program (ERC-CoG MULTIPROSMM grant agreement N725184).