New Generation Molecular Nanomagnets: Experiment and Theory

Kuduva R. Vignesh[a]*

[a]*Department of Chemistry, Indian Institute of Technology Bombay, Mumbai-400076.*

krvignesh245@gmail.com

Abstract

Certain mononuclear/polynuclear complexes are capable of retaining their magnetization even in the absence of magnetic field which gives rise to magnetic hysteresis at a molecular level and an ability to act as magnets below their blocking temperature (T_B) and these molecules are termed Single Molecule Magnets (SMMs).[1] I will discuss about the synthesis and modeling of spin-Hamiltonian parameters (such as magnetic exchange coupling (*J*), zero-field splitting (*D*) and *g*–tensors) in transition metal, lanthanide (Ln), mixed transition metal-lanthanide (3d-Ln) and radical-bridged metal complexes using both experimental and computational tools to understand their molecular magnetic behaviour (Figure a and b). Recently, some new types of complexes have been reported and called Single Molecule Toroics (SMTs), which are defined as molecules that display a toroidal magnetic state that can potentially be used in multiferroic materials. The first example of {3d-Ln^{III}} SMT, a heptanuclear cluster containing Cr^{III} linked to two Dy_3 triangles showed a rare ferrotoroidically coupled ground state, consisting of two con-rotating toroidal moments localised on the Dy_3 triangular rings (Figure c) was reported by us.[2] Also, such a con-rotating ferrotoroidal ground state behaviour in Terbium (III) and Holmium (III) examples and extend the possibility of observing toroidal behaviour in non-Dysprosium (III) complexes for the first time were proven by me will be discussed.[3] Both SMMs and SMTs have several exciting potential applications have since been envisaged, such as high density information storage devices, quantum computing and spintronics devices.[4]

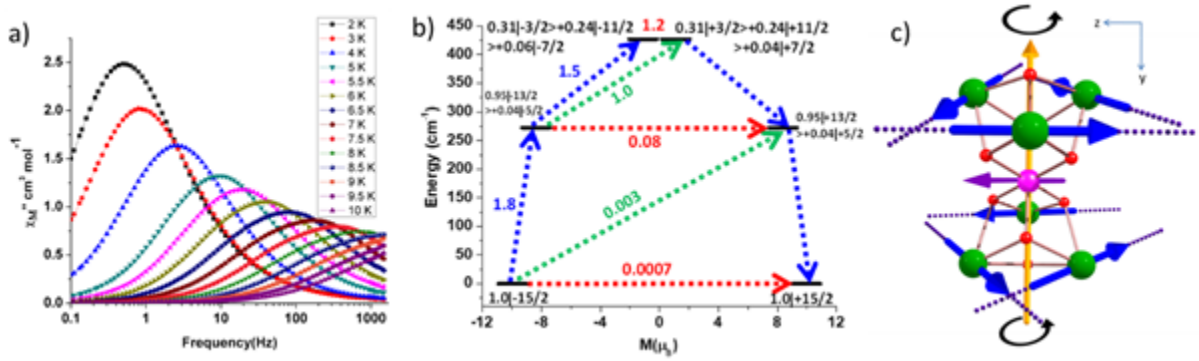

Figure. a) Frequency and temperature dependence of χ_M" for a {$Co^{III}_2Dy^{III}_2$} SMM; *Ab initio* computed b) magnetic relaxation of a {$Co^{III}_2Dy^{III}_2$} SMM and c) orientation of the magnetic anisotropy axes in the ground Kramers doublet on each Dy site (dotted lines and blue arrows) of {$Cr^{III}Dy^{III}_6$} SMT.

References:

1) a) Gatteschi, D.; Sessoli, R.; Villain, J., *Molecular Nanomagnets*. Oxford University Press, Oxford: **2006**; b) Woodruff, D. N.; Winpenny, R. E. P.; Layfield, R. A., *Chem. Rev.* **2013,** *113*, 5110-5148.
2) Vignesh, K. R.; Soncini, A.; Langley, S. K.; Wernsdorfer, W.; Murray K. S.; Rajaraman, G. *Nat. Commun.*, **2017**, *8*, 1023.
3) Vignesh, K. R.; Langley, S. K.; Swain, A.; Moubaraki, B.; Damjanović, M.; Wernsdorfer, W.; Rajaraman, G.; Murray, K. S. *Angew. Chem., Int. Ed.,* **2018**, *57*, 779–784.
4) a) Gatteschi, D., *Adv. Mater.* **1994,** *6*, 635-645. b) Leuenberger, M. N.; Loss, D., *Nature* **2001,** *410*, 789-793. c) Bogani, L.; Wernsdorfer, W., *Nat. Mater.* **2008,** *7*, 179-186.