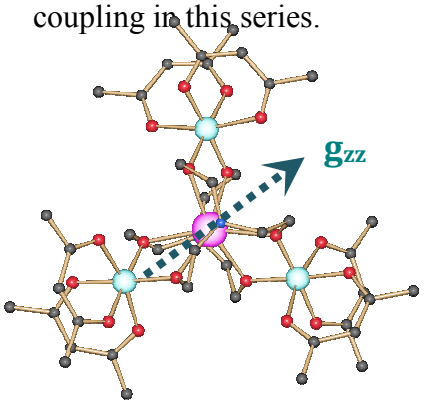
New theoretical perspectives on the Magnetic coupling in {3d-4f} Molecular Nano Magnets

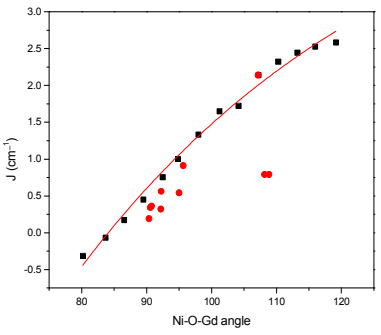
Saurabh Kumar Singh, Gopalan Rajaraman

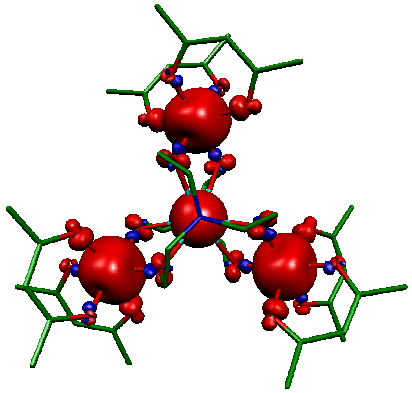
Indian Institute of Technology Bombay, Powai, Mumbai-400076

ssingh@chem.iitb.ac.in

Abstract: Molecular Nano Magnets is a wide area encompassing organic radicals, antiferromagnetic wheels, Single Molecule Magnets (SMMs) to Single chain Magnets (SCMs). Among others, SMMs have been widely studied and these are the molecules which in fact retain magnetization in absence of magnetic field.[1] These SMMs have many potential applications ranging from high-density information storage devices to solid states Q-bits in quantum computing. Despite more than a decade effort, synthesising novel SMMs with the barrier height reaching towards room temperature is still a challenging task. In recent years, an alternative way has been proposed where highly anisotropic 4f ions have been incorporated in cluster aggregation with 3d metals. These {3d-4f} clusters[2] are the appealing candidate for SMMs. Despite extensive experimental reports, theoretical studies are scarce and here we are attempting to study these molecules using density functional methods. We performed density functional calculation and *ab-initio* CASSCF calculations on series of dinuclear complexes of {3d-4f} system[3] and these complexes are the building units of larger polynuclear clusters. We have computed the spin Hamiltonian parameters (magnetic exchange *J*, g tensors, anisotropy etc) to understand the magnetic properties of these clusters and to gain insight in the mechanism of coupling in this series.







References

1. Sessoli, R; Gatteschi, D.; Caneschi, A.; Novak, M. A. *Nature.*, **1993**, *365*, 141.
2. Seesoli, R.; Powell, A. K. *Coord.Chem.Rev.*, **2009**, *253.*
3. Singh, S. K.; Tibrewal, N. K. Rajaraman, G. *Dalton Trans.*, **2011**, *40*, 10897.