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Diplomas

1999: B.Sc., Rajah Serfoji Government College, Thanjavur, India
2001: M.Sc., Bharathidasan University, Trichirappalli, India
2004: Ph.D., University of Manchester, Manchester, U.K

Career summary

2005-2007:	Postdoctoral research: Postdoctoral research: *Prof. P. Comba*, University of Heidelberg, Heidelberg, Germany
2007-2009:	Marie-Curie postdoctoral research: *Prof. D. Gatteschi, Prof. R. Sessoli and Prof. A. Caneschi,* University of Florence, Florence, Italy
2009-2014:	Assistant professor, Department of Chemistry, IIT-Bombay, India
2014-2018:	Associate professor, Department of Chemistry, IIT Bombay, India
2018-present:	Professor, Department of Chemistry, IIT Bombay, India

Selected publications:

1. "*Record high magnetic exchange and magnetization blockade in Ln2@C79N (Ln = Gd(III) and Dy(III)) molecules: a theoretical perspective*", M. K. Singh, N. Yadav, G. Rajaraman, *Chem. Commun.*, **2015**, *51*, 17732-17735.
2. "*An air-stable Dy (III) single-ion magnet with high anisotropy barrier and blocking temperature*", S. K. Gupta, T. Rajeshkumar, G. Rajaraman, R. Murugavel, *Chem. Sci.*, **2016**, *7*, 5181-5191.
3. "*Deciphering the origin of giant magnetic anisotropy and fast quantum tunnelling in Rhenium(IV) single-molecule magnets*", S. K. Singh, G. Rajaraman, *Nat. Commun.*, **2016**, *7*, 10669.
4. "*Ferrotoroidic ground state in a heterometallic Cr Dy 6 complex displaying slow magnetic relaxation*", K. R. Vignesh, A. Soncini, S. K. Langley, W. Wernsdorfer, K. S. Murray, G. Rajaraman, *Nat. Commun.*, **2017**, *8*, 1023.
5. " *Probing the origin of the giant magnetic anisotropy in trigonal bipyramidal Ni(II) under high pressure*", Rajaraman and Murrie and co-workers, *Chem. Sci.*, **2018**, *9*, 1551-1559.
6. " *Deciphering the origin of variation in the spin ground state and oxidation state of a {Mn19} cluster on a Au(111) surface: is the Au(111) surface innocent?*", R. Nabi, G. Rajaraman, *Chem. Commun.*, **2019**, *55*, 8238.

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Role of Molecular Modelling in the Design and Development of Molecular Magnets

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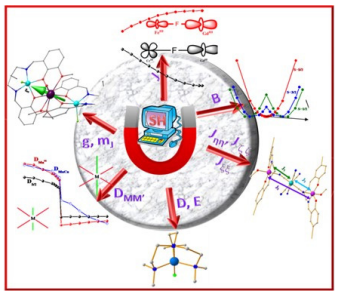
Molecular magnetism is one of the vastly growing research fields with an aim to design the molecules and materials with tunable magnetic and electronic properties.[1] Their synthesis, characterization and implementation as devices which creates lively crossroad among chemistry, physics and material science: a multidisciplinary research field. These molecules have wide-spread potential applications ranging from magnetic storage devices, spintronics, Q-bits in quantum computing to magnetic coolants.[2] Single-molecule magnets (SMMs) are the molecules which show slow relaxation of magnetization below the critical temperature and exhibit hysteresis loop similar to classical magnets. SMMs offer key advantage over classical magnets due to their light-weight, solubility and multifunctional behaviour. Theoretical tools are indispensable in this arena[2] for understanding the observed magnetic properties. The strength of these methods is not only limited rationalization but also to predict novel molecules which can exhibit superior magnetic properties. In this presentation, I will research effort undertaken in our group towards achieving this goal.[2] The second important aspect that needs to be addressed is the nature of surface that often alters the magnetic properties. With one example, we show how theoretical studies can offer insight into the nature of magnetic interactions present in molecular magnets on surface.[3]



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[2] S. K. Singh, G. Rajaraman, *Nature Commun.*, **2016**, 7, 10669; S. K. Gupta, T. Rajeshkumar, G. Rajaraman, R. Murugavel, *Chem. Sci.*, **2016**, 7, 5181-5191; M. K. Singh, N. Yadav, G. Rajaraman, *Chem. Commun.*, **2015**, 51, 17732-17735.; T. Gupta, G. Rajaraman *Chem. Comm.*, **2016**, 52, 8972.
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