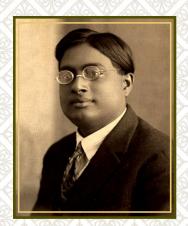


## S. N. Bose National Centre for Basic Sciences



# Bose Colloquium

28th February, 2019 | 04:00 pm | Fermion Hall

### Speaker

#### Prof. S. Ramasesha

Solid State and Structural Chemistry Unit Indian Institute of Science, Bangalore

#### Title

Modeling magnetic anisotropy in molecular magnets

#### **Abstract**

In the emerging field of Molecular Magnetism two very important aspects are (i) solving the exchange Hamiltonian and (ii) computing molecular magnetic anisotropy constants D<sub>M</sub> and E<sub>M</sub>. We introduce a method for spin and spatial symmetry adapted technique for solving the exchange Hamiltonian. We present a theoretical approach to calculate these constants from single-ion anisotropies [1]. We treat anisotropy Hamiltonian (H<sub>2</sub>) as perturbation to exchange Hamiltonian (H<sub>2</sub>). To get anisotropy constants (from H<sub>2</sub>) in a chosen spin-sector (say, ground-state spin) one has to first solve He to obtain eigenstate(s) with required total spin. For large system solving He can pose a serious challenge. To overcome these problems, we here employ a new hybrid technique based on Valence Bond and Constant Ms basis, developed by us, which exploits both spin and spatial symmetries to (a) block-diagonalize He to smaller dimensions and (b) designate eigenstates with appropriate total spin [2]. Spins in molecular magnets can experience both anisotropic exchange interactions and on-site magnetic anisotropy. In this talk, I will also discuss the effect of strong single ion anisotropy as well as the effect of exchange anisotropy on the molecular magnetic anisotropy both with and without on-site anisotropy will be discussed. When both the anisotropies are small, we find that the axial anisotropy parameter  $D_{_{\mathrm{M}}}$  in the effective spin Hamiltonian is the sum of the individual contributions due to exchange and on-site anisotropies. We find that even for axial anisotropy of about 15%, the low energy spectrum does not correspond to a single parent spin manifold but has intruders states arising from other parent spin. In this case the low energy spectrum cannot be described by multiplet states arising from a single approximate total spin state.

#### REFERENCES

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