S. N. Bose National Centre for Basic Sciences

Bose Colloquium

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Speaker

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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_M and E_M. 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_a) as perturbation to exchange Hamiltonian (H_e). To get anisotropy constants (from H_a) 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_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.

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