Theoretical modeling of spectroscopic properties of Ni^{2+} ions in Haldane gap systems - case study: Y_2BaNiO_5

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Modeling of spin Hamiltonian (SH) parameters enables correlation of crystallographic, spectroscopic, and magnetic data for transition ions in crystals [1]. As a case study we consider Ni^{2+} ($3d^8$) ions in the Haldane gap system Y_2BaNiO_5 [2]. In the first stage, using the crystallographic data [3] and the point-charge model (PCM) [1b] the crystal field parameters (CFPs) are estimated for Ni^{2+} in Y_2BaNiO_5. The CFPs serve as input for the high-order perturbation theory microscopic spin Hamiltonian (MSH) expressions [1b] for the zero-field splitting parameters (ZFSPs): *D* and *E*. In the second stage, the superposition model (SPM) analysis of CFPs as well as ZFSPs is carried out using the SPM expressions derived by us for the pertinent geometry around the orthorhombic and axial sites in various Haldane gap materials. In the third stage, the SPM-derived CFP sets are used as input for the crystal field analysis package CFA/MSH [1a] to obtain more accurate of MSH modeling of ZFSPs. An extensive literature search is ongoing to extract: (i) crystallographic data as input for SPM calculations, (ii) experimental ZFSPs for Ni^{2+} ions in the Haldane gap materials, and (iii) model parameters to serve as input for SPM/CFP and SPM/ZFSP calculations. The data obtained by various techniques are systematically categorized to enable their meaningful analysis and comparison. The aims of this project are: (i) to verify the experimental results on the single ion anisotropy, (ii) to provide deeper understanding of the nature of the Haldane gap, (iii) to explain or disprove the observed maximal orthorhombic distortion ($|\lambda| = |E/D| = 1/3$, see, e.g. [2,3]. Important preliminary finding indicate that the project's results may lead to reanalysis of earlier magnetic studies and basic concepts as well as novel ideas on the nature of the Haldane gap in YBNO, NENP and related systems.

References

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