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Dynamic Compensation Temperature in the Mixed Spin-1/2 and Spin-3/2 Ising Model in an Oscillating Field on Alternate Layers of Hexagonal Lattice

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The two-sublattice mixed-spin Ising systems have been intensively studied both experimentally and theoretically due to reason that these systems mainly related to the potential technological applications in the area of thermomagnetic recording [1]. Moreover, the mixed-spin Ising systems have less translational symmetry than their single spin counterparts; hence exhibit many new phenomena that cannot be observed in the single-spin Ising systems, and the study of these systems can be relevant for understanding of bimetallic molecular systems based magnetic materials [2]. In this work, the dynamic behavior of a mixed spin-1/2 and spin-3/2 Ising model [3] with a crystal-field interaction in the presence of a time-varying magnetic field on a hexagonal lattice is studied by using the Glauber-type stochastic dynamics. The lattice is formed by alternate layers of spins σ=1/2 and S=3/2. For this spin arrangement, any spin at one lattice site has two nearest-neighbor spins on the same sublattice, and four on the other sublattice. The intersublattice interaction is antiferromagnetic. First, we study time variations of the average magnetizations in order to find the phases in the systems, and the reduced temperature dependence of the dynamic magnetizations to obtain the dynamic phase transition (DPT) points as well as to characterize the nature (continuous and discontinuous) of transitions. Then, the behavior of total dynamic magnetization as a function of the reduced temperature is investigated to find the dynamic compensation temperature which is interesting phenomenon with important technological applications such as the high density magneto-optical recording [4,5]. Dynamic phase diagrams are calculated for both DPT points and dynamic compensation temperature. According to values of Hamiltonian parameters, besides the paramagnetic (p), antiferromagnetic (af) and antiferrimagnetic (i) phases, the i+af, i+p and af+p mixed phases, and the compensation temperature or L-type behavior [6] in Néel classification nomenclature exist in the system.

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AC09

Theoretical Study of Exchange Couplings in Mn_4 Single-molecule Magnets

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Single-molecule magnets (SMMs), individual molecules that can function as magnets below their blocking temperature (T_B), have received tremendous attention due to both their particular physical properties, such as macroscopic quantum tunneling [1], and their potential applications, such as quantum bits for quantum computing [2]. However, the current record of the T_B of SMMs is only several degrees Kelvin. This temperature is far too low for practical use. The increase of T_B requires enhancement of the ground-state spin (S) and the axial zero-field splitting parameter (D). In turn, S and D are determined by exchange couplings between transition-metal (TM) ions through ligands in SMMs [3]. While the previous theoretical studies have tried to calculate important physical quantities of SMMs, a description of the mechanism of exchange couplings between TM ions in SMMs is still missing [3].

On the basis of density-functional theory (DFT) calculations, we investigate the mechanism of exchange couplings and the role of ligands in controlling exchange-couplings in distorted-cubane $[Mn^{4+}Mn^{n+}{}_3(\mu_3\text{-}L)_3(\mu_3\text{-}X)(RCOO)_3(L1,L2)_3]$ (n = 2–4; L, X, R, L1, and L2 = various) SMMs to support for designing SMMs with high T_B. Each exchange coupling between the Mn spin centers is analyzed in terms of exchange integrals (J values), orbital overlap integrals (T values) and natural orbitals. It was found that couplings $Mn^{4+}/\mu_3\text{-}L/Mn^{n+}$ couplings mainly control the whole magnetic properties. These couplings result from decentralization of d electrons from Mn^{n+} ions to the Mn^{4+} ion through μ_3-L ligands, depending on charge and spin states of manganese ions that can be controlled by ligand substitutions.

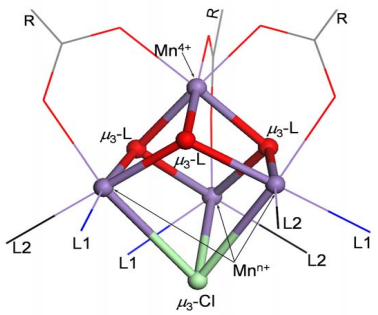

Fig. 1. A schematic geometric structure of Mn4 SMMs.

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