EP10

Electronic Structures and Noncollinear Magnetism in GdB_4

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Among the rare-earth teraborides, GdB_4 is relatively less studied due to the difficulty in synthesis of its single crystal. Moreover, the high absorption of neutron by Gd and B atoms in GdB_4 makes it difficult to study its magnetic structure. The susceptibility measurements on GdB_4 indicate that magnetic moments of Gd lie in the basal plane, and according to the recent neutron polarimetry measurement, the magnetic moments in the basal plane have noncollinear spin arrangement. But the origin of noncollinear magnetic structure is still unknown. Motivated by all these considerations, we have investigated electronic and magnetic properties of GdB_4 employing the first-principles full potential linearized augmented plane wave (FLAPW) band method in the generalized-gradient approximation including the Coulomb correlation (GGA+U). We have analyzed both the collinear and the noncollinear magnetic state in GdB_4. All the possible noncollinear magnetic configurations proposed in experiments are discussed in our theoretical work. The results show that the clock-wise noncollinear magnetic moment arrangement in plane is to be the ground state. But the stabilization energy of the noncollinear state with respect to the collinear state is very minor. Further, the energy difference between different noncollinear magnetic configurations is even smaller, which suggests the possibility of a more complex noncollinear magnetic ground state in GdB_4.

EP11

Effects of a Crystal Field on the Magnetic Properties of a Spin-1 Ising System

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The magnetic properties such as the hysteresis loops, susceptibility and magnetization of a spin-1 Ising system and by using the effective field theory with a probability distribution technique that accounts for the self spin correlation functions are studied. The effects of the crystal field on the magnetic properties are discussed and numerical results are performed and analyzed for the cases of the honeycomb, square and simple cubic lattices. A number of interesting phenomena such as the shape of the hysteresis loops and the susceptibility have been found.

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