Magnetic ordering of rare-earth compounds: first-principles studies

CHUN-GANG DUAN, University of Nebraska Lincoln, R. F. SABIRIANOV, L LIU, W.N. MEI, UNO, P.A. DOWBEN, UNL, E.Y. TSYMBAL, UNL — We report a systematic theoretical study on the magnetic ordering in heavy rare-earth compounds with face-centered cubic structure. Based on first-principles total energy calculations of Gd monopnictides, we deduced the exchange interaction parameters of these systems from fitting the total energies of different magnetic configurations to those computed from the Heisenberg model. Then we demonstrated the formation of different magnetic structures in these compounds by using the Monte Carlo simulations. The so obtained Curie (Néel) temperatures agreed well with experiments. Detailed analysis on the trend of exchange parameters changing with anion sizes and distances between neighboring magnetic sites clearly demonstrate the co-existence of RKKY type metallic exchange interactions and anti-ferromagnetic superexchange interactions. We then propose a Bethe-Slater type curve which can qualitatively explain the behaviors of the exchange parameters in Gd monopnictides.

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