First-principles calculations of the magnetic hyperfine field at Cd sites in RECd (RE = rare-earth element)

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Binary magnetic compounds based on rare-earth (RE) elements of the type REX, where X is a transition metal, with the simplest stoichiometry and crystalline cubic structure, are isostructural systems with different RE constituents, which differ only slightly in the crystallographic properties, but strongly in the magnetic properties. They thus offer excellent conditions for the separation of the magnetic from other solid-state parameters and permit the magnetism studies. However, in most RE compounds and, particularly when X=Cd, details of the magnetic structure at an atomic scale are not available mainly because is not possible to use neutron diffraction to investigate them. In this paper, the magnetic hyperfine field (m_{hf}) at Cd sites in RECd compounds was studied by first-principles calculation. These compounds crystalizes in the CsCl prototype cubic structure (Pm-3m space-group) and order ferromagnetically below the Curie temperature with exception of PrCd, which presents antiferromagnetism. Recently, it was observed an unexpected transition in the m_{hf} at ^{111}Cd in DyCd below 40 K, when m_{hf} vanishes [1]. We have used the density functional theory framework with full potential Augmented Planes Waves plus local orbitals (APW+lo) method embodied in the WIEN2k code to simulate electronic structures of the ferromagnetic and antiferromagnetic crystal cells in these compounds. For the exchange-correlation effects we chose local density approximation. The m_{hf} at Cd sites and the formation energy were calculated for each compound as well as the density of states were obtained. Results of m_{hf} are in very good agreement (less than 10%) with the experimental values previously reported [1]. Interestingly, for DyCd the energy for the formation of the antiferromagnetic ordering with (π, π, 0) structure is smaller than that for the ferromagnetic and others possible antiferromagnetic phases. As far as we know, it is the first time that such an excellent agreement between the calculated and experimental m_{hf} at Cd sites is observed. Moreover, this results is even more important because the calculations were fully variational without the use of the Hubbard model which takes into account the on-site correlation of 4f electrons.

[1] F. H. M. Cavalcante, O. F. L. S. Leite-Neto, M. Forker et. al., to be published.