First-principles study of magnetic interactions in 3d transition metal-doped phase-change materials

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ABSTRACT

Recently, magnetic phase-change materials have been synthesized experimentally by doping them with 3d transition metal impurities. Here, we investigate the electronic structure and the magnetic properties of the prototypical phase-change material $Ge_2Sb_2Te_5$ (GST) doped with V, Cr, Mn and Fe by density functional calculations [1]. Both the supercell method and the coherent potential approximation (CPA) are employed to describe this complex substitutionally disordered system. As regards the first approach, we consider a large unit cell containing 1000 sites to model the random distribution of the cations and of the impurities in doped cubic GST. Such a large-scale electronic structure calculation is performed using the program KKRnano, where the full potential screened Korringa-Kohn-Rostoker Green's function method is optimized by a massively parallel linear scaling (order-N) all electron algorithm [2,3]. Overall, the electronic structures and magnetic exchange coupling constants calculated by KKRnano agree quite well with the CPA results. We find that ferromagnetic states are favorable in the cases of V and Cr doping, due to the double exchange mechanism, whereas antiferromagnetic superexchange interactions appear to be dominant for Fe- and Mn-doped GST. The ferromagnetic interaction is particularly strong in the case of Cr. As a result, high Curie temperatures close to room temperatures are obtained for large Cr concentrations of 15 %.

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