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Curie temperatures and exchange interactions in diluted group-IV magnetic semiconductors

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Abstract

Effective exchange interactions between magnetic atoms in GeMnCr alloys are obtained from the first principles by mapping total energies associated with rotations of magnetic moments onto the effective classical Heisenberg Hamiltonian. The calculated Curie temperature increases with Mn concentration but decreases linearly with increasing Cr content in a good agreement with a recent experiment.

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Keywords: Magnetic semiconductors; Curie temperature; Exchange interactions; First principles

The diluted magnetic semiconductors (DMS) exhibit long-range ferromagnetism mediated by holes in the valence band of the host semiconductor and thus represent new materials with promising applications in spintronics [1]. Most of the effort in the past has focused on III–V compounds, but recently ferromagnetism in group IV semiconductors doped with Mn was also found [2].

In the present paper, we describe magnetic properties and Curie temperatures of $Ge_{1-x}Mn_x$ and $Ge_{1-x-y}Mn_xCr_y$ from the first principles using tight-binding linear muffin-tin orbital method combined with the coherent potential approximation (CPA) [3] to describe the substitutional disorder due to magnetic impurities. The calculated total energies are then mapped onto an effective Heisenberg Hamiltonian (HH) [4]

$$H = -\sum_{i \neq j} J_{ij} \mathbf{e}_i \cdot \mathbf{e}_j \qquad (1)$$

from which the Curie temperature is estimated via statistical mechanical methods (mean-field approximation, Monte Carlo simulations, etc.). Here, $\mathbf{e}_i$ and $\mathbf{e}_j$ are unit vectors of the local magnetic moments at sites i and j, and J_{ij} denote the random effective pair exchange interactions between atoms carrying magnetic moments (Mn and Cr). The Heisenberg parameters J_{ij} are obtained in terms of the magnetic force theorem [4] by (i) directly evaluating the change of energy associated with a constrained rotation of the spin-polarization axes in atomic cells i and j in the framework of the CPA, and (ii) using the vertex-cancellation theorem [5]. The mapping to the effective HH is based on the adiabatic approximation which is justified for atoms with large exchange splitting like e.g. Mn. Exchange interactions J_{ij} reflect both the geometric structure (lattice geometry, alloy composition) as well as different electronic properties of various impurities. Because we have an explicit expression for pair exchange interactions between different magnetic atoms [4], we can also estimate their long-range and oscillatory behavior as well as their dependence on the alloy composition. The detailed knowledge of exchange interactions as a function of material parameters is relevant for a deeper

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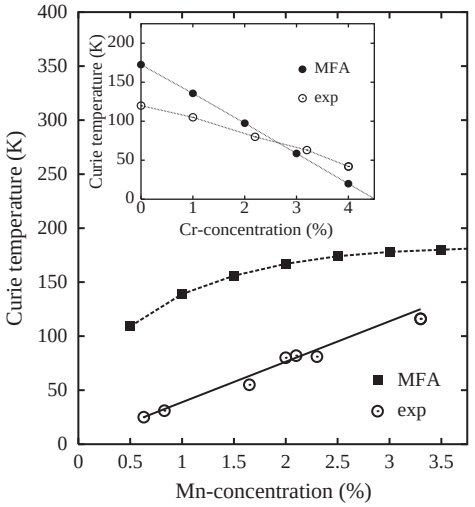

Fig. 1. Calculated Curie temperatures of $Ge_{1-x}Mn_x$ and $Ge_{0.975-y}Mn_{0.025}Cr_y$ (inset) alloys in the mean-field approximation compared to the experiment [2,7].

understanding of the nature of magnetic interactions in DMS. In particular, it is known [6] that the disorder leads to the exponential rather than to the power-law damping characteristic for the RKKY oscillations.

The calculated total magnetic moment per Mn-atom is 3 μ_B for $Ge_{1-x}Mn_x$ and Curie temperatures (T_c) increase monotonically with x (see Fig. 1) in a good agreement with experiment [2]. There is no long-range ferromagnetism for $Ge_{1-x}Cr_x$ alloys and T_c for $Ge_{0.975-y}Mn_{0.025}Cr_y$ decreases linearly with increasing Cr content in an agreement with experiment [7]. The experiment indicates that only a part of impurities is magnetically active and that the number of carriers is smaller than the number of Mn atoms. These facts explain some quantitative differences between theory and experiment. Calculations confirm the predicted exponential damping [6] of exchange interactions due

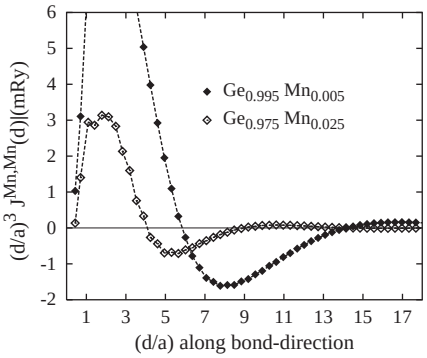

Fig. 2. Exchange interactions between Mn atoms in $Ge_{1-x}Mn_x$ alloys as a function of the distance along the bond-direction.

to the substitutional disorder while their ferromagnetic character is preserved for distances larger than the average distance between Mn impurities (see Fig. 2). Periods of damped oscillations increase with decreasing number of carriers, i.e., with Mn content.

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