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First-principles study of the thermal properties of half-metallic ferromagnetic systems

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ABSTRACT

The origin of the half-metallicity is different in diluted magnetic semiconductors and Heusler alloys. I briefly review our earlier work on (GaMn)As and (GaMn)N focusing on the relation between the half-metallicity and the strength of the interatomic exchange interactions. This relation is governed by the properties of the valence-band holes. In Heusler alloys the factors determining the thermal behavior are distinct. Here the relation between half-metallicity and the longitudinal fluctuations of atomic moments is considered. The temperature dependence of the Ni magnetization in NiMnSb is studied.

1. Introduction

The half-metallicity is an interesting state of magnetic systems where the electronic structure of one of the spin-subsystems is metallic whereas the electronic structure of the other is semiconducting. Since the half-metallic materials are characterized by a 100% spin-polarization of the electronic states at the Fermi level they are promising candidates for the applications in the spintronic devices utilizing the spin degree of freedom.

Among the half-metallic materials attracting most research attention are the diluted magnetic semiconductors (DMS) and Heusler alloys. Since the spintronics devices should be operative at room temperature the Curie temperature of the materials suitable for applications must exceed the room temperature considerably. The value of the Curie temperature is determined by exchange interactions in the electron system. The understanding of the mechanisms of the exchange interactions in the half-metallic materials is of primary importance for both fundamental physics and applications.

2. Half-metallic (GaMn)As

The half-metallicity of the DMS and Heusler alloys has different nature. In the DMS, we deal with the systems that, in the absence of the impurities, are semiconducting and nonmagnetic. The origin of the gap between occupied and empty electron states in this case does not have a magnetic character and is a consequence of the hybridization of the electron states of the nonmagnetic matrix. A magnetic impurity contributes differently to the two spin channels of the electron structure. The formation of a half-metallic state is connected with establishing of the long-range magnetic order of impurity moments.

Taking as an example (GaMn)As with Mn impurities substituting Ga atoms in GaAs one finds (Fig. 1) that a strongly spin-polarized Mn atom contributes five additional states into the energy region of the valence band of GaAs and only four additional electrons. Therefore, there is one hole per Mn atom at the top of the valence band. The minority-spin 3d states of the Mn atom are shifted to higher energies by the intra-atomic Mn exchange splitting. They are empty and do not overlap with the valence band of GaAs. If the Mn moments are ferromagnetically ordered the majority-spin electronic structure of (GaMn)As is metallic whereas the minority-spin electronic structure remains semiconducting.

The frozen-magnon calculations [1] show that the ferromagnetic half-metallic state corresponds to the minimum of the total energy of the system. These calculations allow the mapping of the system on an effective Heisenberg Hamiltonian and the estimation of the Curie temperature T_C. In Fig. 2 we show the dependence of T_C of (GaMn)As on continuous variation of the electron number [2]. The presence of the holes plays crucial role in the formation of the effective ferromagnetic interatomic exchange interactions. With decreasing number of holes the Curie

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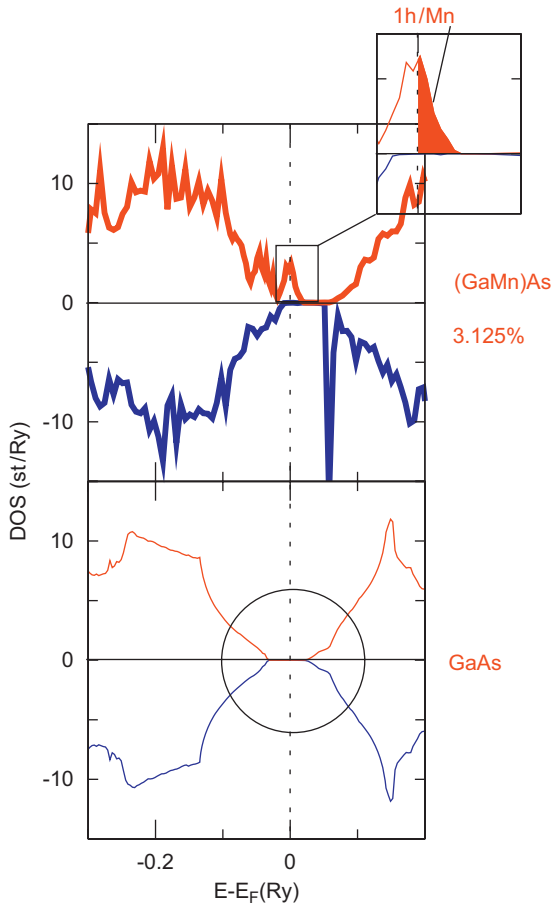

Fig. 1. (Color online) Lower panel: The density of states of semiconductor GaAs. Upper panel: The density of states of the diluted magnetic semiconductor (GaMn)As. The calculation is performed for the ferromagnetic ordering of the Mn moments. The substitution of 3% of Ga atoms by Mn atoms results in a half-metallic state with semiconducting spin-down channel and with exactly one hole per Mn atom in the spin-up channel.

temperature decreases. For completely filled valence band and empty conduction band ($n=1$ in the figure) the leading interatomic exchange interactions are antiferromagnetic.

Two features of the holes are crucial for mediating the exchange interaction between Mn atoms: the exchange interaction with magnetic impurity and the delocalization from the impurity. Both components are necessary since neither a hole localized on the impurity atom nor the holes that do not interact with impurities can mediate the interaction between impurities [3]. These two properties of the holes are competitive with each other since increasing delocalization of the holes from the impurity leads to decreasing exchange interaction with the

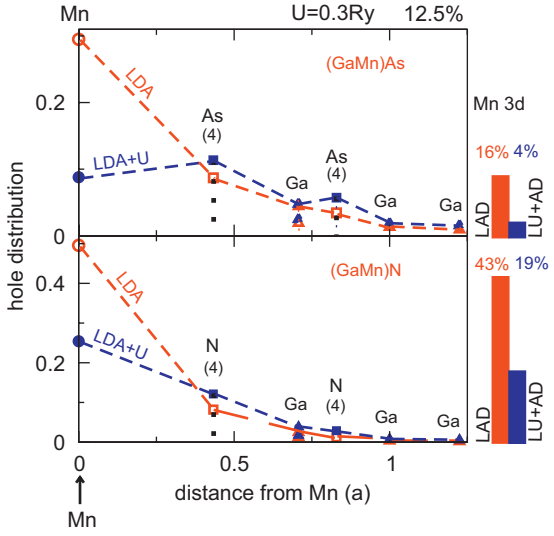

Fig. 3. The hole distribution in (GaMn)As and (GaMn)N with 12.5% of Mn. The calculations are performed within local density approximation (LDA) and LDA+U approaches. The LDA+U scheme assumes stronger on-site Coulomb correlations of the Mn 3d electrons. In LDA+U, the part of the hole localized on Mn atoms decreases strongly compared to LDA that corresponds to increased delocalization of the hole from the impurity. On the other hand, the decreased contribution of the Mn 3d states to the hole (histograms in the right part of the figure) can be treated as decreasing exchange interaction between impurity and hole.

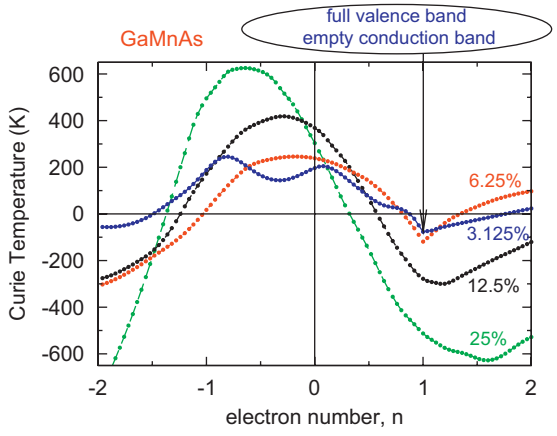

Fig. 2. (Color online) The dependence of the Curie temperature on the electron number. The mean-field value of T_C is proportional to the sum of the interatomic exchange parameters. The negative value of T_C means prevailing antiferromagnetic exchange interactions and the instability of the ferromagnetic structure. $n=0$ corresponds to the nominal number of electrons giving 1 hole per Mn atom. For low Mn concentrations of 3% and 6% $n=1$ corresponds to the completely filled valence band and completely empty conduction band. For larger concentrations there is an overlap between the valence and conduction bands.

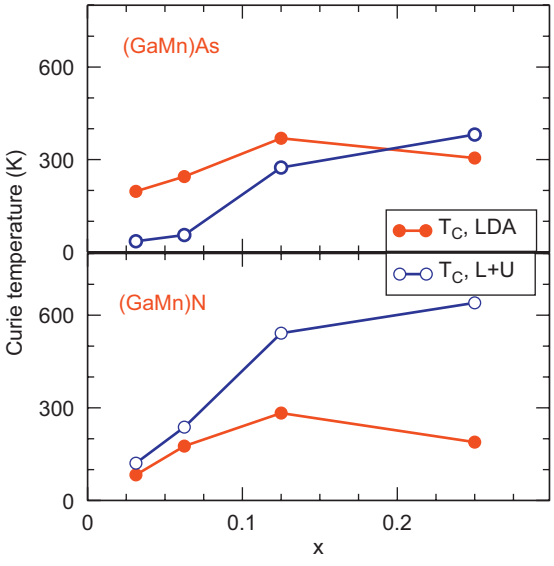

Fig. 4. The dependence of the calculated Curie temperature of (GaMn)As and (GaMn)N on the Mn concentration calculated within LDA and LDA+U (denoted with L+U) approaches. Since the compromise between the delocalization of the hole from impurity and the exchange interaction with impurity is different for the two systems the dependence of T_C on U is also different.