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ORIGINAL PAPER

Ab Initio, Mean Field and Series Expansions Calculations Study of Structural, Electronic and Magnetic Properties of MnAs

R. Masrour · E. K. Hlil · M. Hamedoun · A. Benyoussef · O. Mounkachi · H. El Moussaoui

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Abstract The self-consistent ab initio calculations, based on density functional theory (DFT) approach and using full-potential linear augmented plane wave (FLAPW) method, are performed to investigate both electronic and magnetic properties of the MnAs compounds. Polarized spin and spin-orbit coupling are included in calculations within the framework of the ferromagnetic state between two adjacent Mn atoms. The ferromagnetic and antiferromagnetic energies of MnAs systems are obtained. Magnetic moment considered to lie along (001) axes is computed. The obtained data from ab initio calculations are used as input for the high-temperature series expansion (HTSE) calculations to compute other magnetic parameters. The exchange interactions between the magnetic atoms Mn-Mn in MnAs are given using the mean field theory. The HTSEs of the magnetic susceptibility with the magnetic moments in MnAs (m_{Mn}) through the Ising model is given up to the *ten*th order series in $x = J_1(\text{Mn-Mn})/k_B T$. The Néel temperature T_C is obtained by HTSEs of the magnetic susceptibility series combined with the *Padé* approximant method. The critical exponent γ associated with the magnetic susceptibility is deduced as well.

Keywords Electronic and magnetic structure · Magnetic moment · Néel temperature · Exchange interactions

1 Introduction

The candidate material ferromagnetic zincblende (ZB) MnAs [1] suffers from some experimental and theoretical drawbacks [2, 3]. Very recently, Janotti et al. [13] studied the stability of the ferromagnetic and antiferromagnetic phases of zincblende MnN and MnAs compounds within the local density approximation. The theoretical approaches local density approximation (LDA) [4, 5] and the generalized gradient approximation (GGA) [6] are used for MnN and MnAs, respectively. MnAs is a metallic compound that is ferromagnetic below $T_C = 313$ K where the first-order phase transition from hexagonal to orthorhombic is accompanied by a ferromagnetic-paramagnetic transition [7]. In half-metals like MnAs and CrAs, the majority spins are metallic and a gap appears for the minority spins [8]. Galanakis and Mavropoulos [9], motivated by the successful fabrication of ZB CrAs, CrSb and MnAs [10], examined the possibility of half-metallic behaviour in ordered ZB compounds of transition metals V, Cr and Mn with the "sp" elements N, P, As, Sb, S, Se and Te.

In this work, three approaches, self-consistent ab initio calculations, mean field and high-temperature series expansions (HTSEs) calculations, are used to shed light on the

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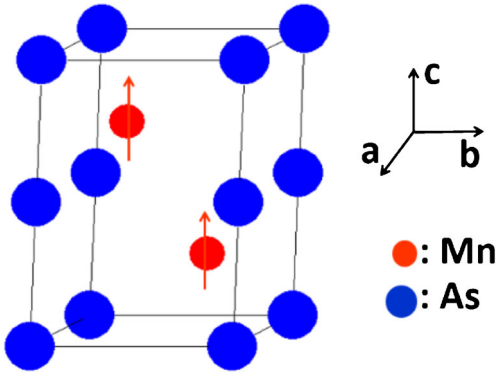

Fig. 1 The structure of MnAs compound as used in calculations

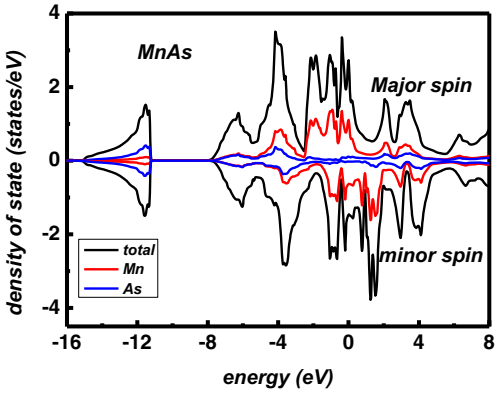

Fig. 2 Total DOS, Cr DOS and Sb DOS from FLAPW calculations

magnetic structure. Firstly, full-potential linear augmented plane wave (FLAPW) calculations based on density functional theory (DFT) principle are performed on MnAs compound. Appropriate polarized spin and spin-orbit coupling as well as ferromagnetic state are considered. Considering computed magnetic moment from FLAPW calculations as input data, we have used the mean field theory to find the first and second exchange interactions between the magnetic atoms Mn-Mn in MnAs compound. Also, the ferro and antiferromagnetic energies are computed. The HTSEs of the magnetic susceptibility of MnAs through the Ising model combined with the *Padé* approximant [11] is studied up to the *ten*th order series in ($\beta = 1/k_{\mathrm{B}}T$). Finally, the Néel temperature is deduced.

2 Electronic Structure Calculations

We used the FLAPW method [12] which performs DFT calculations using the local density approximation. The Kohn-Sham equation and energy functional were evaluated consistently using the FLAPW method. For this method, the space was divided into the interstitial and the non overlapping muffin tin spheres centred on the atomic site. The employed basis function inside each atomic sphere was a linear expansion of the radial solution of a spherical potential multiplied by spherical harmonics. In the interstitial region, the wave function was taken as an expansion of plane waves and no shape approximation for the potential was introduced in this region which is consistent with the full-potential method. The core electrons were described by atomic wave functions which were solved relativistically using the current spherical part; the valence electrons were also treated relativistically in our case. These FLAPW calculations were performed with the crystal structure parameters reported in [13]. Here, polarized spin, spin-orbit coupling as well as the ferromagnetic state were considered for Mn adjacent atoms. The Mn magnetic moments were considered to lie along (001) axes [14].

3 Magnetic Properties of MnAs

3.1 Mean Field Theory

The Hamiltonian of the system is given by the following:

$$H = -\sum_{<i,j>} J_{ij} m_{\,iMn} m_{\,jMn} - h \sum_{i} m_{\,iMn} \tag{1}$$

where h is the external magnetic field, J_{ij} (J_1(Mn-Mn) and J_2(Mn-Mn)) are the first and second exchange interactions between the (Mn-Mn) atoms in MnAs compound (see Fig. 1) and $m_i m_i$ is the magnetic moment of Mn ion located on the ith site. In this work, we consider the nearest-neighbouring (nn)(nn) and next-nearest neighbouring (nnn)(nnn) interactions J_1(Mn-Mn) and J_2(Mn-Mn), respectively. The mean field approximation used in [15] leads to simple relations between exchange integrals J_1(Mn-Mn) and J_2(Mn-Mn) to the critical temperature T_{C} and the paramagnetic Curie temperature θ_{CW}. The expression obtained is as follows:

$$\begin{aligned} \mathbf{J}_1 &= (\mathbf{3}/\,(2m\,(m+2)))\,(\theta_{\mathrm{CW}} + \mathbf{T}_N) \\ \mathbf{J}_2 &= (\mathbf{3}/\,(4m\,(m+2)))\,(\mathbf{T}_N - \theta_{\mathrm{CW}}) \end{aligned} \tag{2}$$

Table 1 The series coefficients for the high-temperature developed susceptibility series bcc lattices for MnAs compounds for Ising model with magnetic moment $m_{\mathrm{Cr}} = 2.82\ \mu_{\mathrm{B}}$

a_0	a_1	$-a_2$	$-a_3$	$-a_4$	$-a_5$	$-a_6$	$-a_7$	$-a_8$	$-a_9$	$-a_{10}$
1	48.97	186.096	693.456	2552.218	9361.419	33810.932	122175.58	440004.23	1580412.22	5664204.831

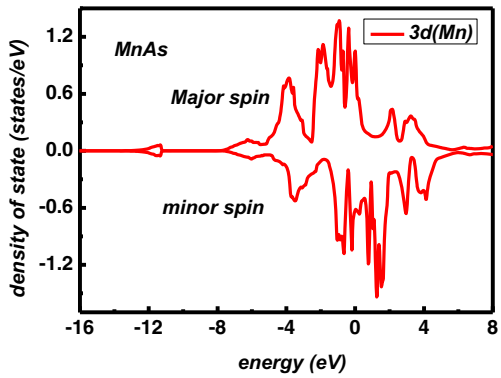

Fig. 3 The l-decomposed DOS of $3d$-like states of Mn in MnAs from FLAPW calculations

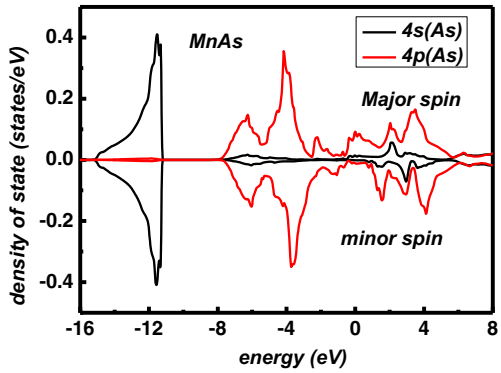

Fig. 4 The l-decomposed DOS of $4s$ and $4p$-like states of Mn in MnAs from FLAPW calculations

where k_B is the Boltzmann's constant, $m = 1.48 \infty_B$ (μ_B is Bohr magnetron), T_C is the Curie temperature and θ_{CW} is the Curie-Weiss temperature.

3.2 High-Temperature Series Expansion

The theoretical method used in this study has been developed in previous papers [16]. Here, we consider a magnetic moment (m) and we use the following function:

$$\chi\,(T) = \sum_{i,j} \langle \vec{S}_i \vec{S}_j \rangle_T = \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} \alpha_l \beta^l \tag{3}$$

With $\alpha_l \approx (J_{sk_1}^{m_1} J_{k_2 k_3}^{m_2} \ldots J_{k_w \perp}^{m_v})[\alpha_l]$

The HTSE method is developed for the magnetic susceptibility $\chi\,(T)$ with arbitrary exchange interactions J_1(Mn-Mn) and J_2(Mn-Mn). The "weight" $[\alpha_l]$ of each graph is tabulated and given in [17]. The $k_1, k_2, \ldots, k_w$ represent the sites surrounding the sites i and j.

$$\chi(\beta) = \beta \sum_{n=0}^{m} \sum_{m=0}^{10} a_m^n y^m x^n \tag{4}$$

With $x = \frac{J_1}{k_B T}$ is the reduced temperature, β is a Boltzmann constant and $y = \frac{J_1}{J_2}$. The coefficients a_m^n given in the magnetic susceptibility of MnAs as a compound are tabulated in Table 1 for the Ising model. The high-temperature series expansions of magnetic susceptibility obtained in the present calculation is directly evaluated from the two rooted diagrams. The high-temperature series expansions of magnetic susceptibility could also be evaluated from the free energy to second order in h and, taking the derivative of the result twice with respect to the field.

4 Results and Discussions

The density of state (DOS) of MnAs deduced from band structure calculations is reported in Fig. 2. Here, the Fermi level is taken as reference. This DOS is dominated by the Mn atom contributions taking place in both occupied states at negative energies and unoccupied states localized at positive energies. As seen, this DOS is not symmetrical with respect to energy axis, pointing out that magnetic moments carried by Mn atoms are ferromagnetically ordered.

The l-decomposed DOS of s, p and $d-$like states, reported in Figs. 3 and 4, provides a more detailed picture and allows to conclude that both Mn contributions have mainly a character of $3d$ band while the projected DOS on As atom is dominated by contributions from $4p$ band. The magnetic moment of Mn is computed as well and found equal to 1.48 μ_B.

We have used the magnetic measurement of Néel temperature and Curie-Weiss reported in [14, 18] to calculate the exchange integrals J_1(Mn-Mn) and J_2(Mn-Mn) by using

Table 2 The Néel temperature, exchange interactions, ferro and ferromagnetic energies and the critical exponents of MnAs for Ising model

System	T_N (K) HTSE	T_N (K) experiment [14]	J_1(Mn-Mn) (K)	J_2(Mn-Mn) (K)	Critical exponents γ	E_{FM}(K) ab-initio calculations	E_{AFM}(K) ab-initio calculations
MnAs compounds	322	318	171.148	−13.979	1.36 ± 0.02	±0.2976542336 10^{-13}	−0.2976540249 10^{-13}

the mean field theory. The obtained values are given in Table 2. The high-temperature series expansion (HTSE) extrapolated with Padé approximants method is known to be a convenient method to provide a valid estimate of the critical temperatures for real system. By applying this method to the magnetic susceptibility $\chi(T)$, we have estimated the Néel temperature T_C for MnAs. The Padé approximant analysis of the magnetic susceptibility is used to estimate the Néel temperature of MnAs compound. The obtained value is close to those obtained in [19–22]. The Néel temperature corresponds to the simple pole of $[\chi]^{1/2}$. The obtained values are gathered in Table 2. In comparison with those obtained by Monte Carlo simulations in bulk case [23–28], these values are close to those given in general universality principles. Also, the critical exponent γ associated with the magnetic susceptibility $\chi \approx (T - T_C)^{-\gamma}$ is computed for different values of Padé approximant for the Ising model (see Table 2).

5 Conclusions

FLAPW calculations were performed to investigate both electronic and magnetic structures for MnAs compound. They evidence that the DOS of Mn atoms originate essentially from contributions of $3d$ bands. The projected DOS on As atoms is dominated by contributions from the $4p$ band. Magnetic moments carried by Mn atoms were computed as well and used as input data for HTSE calculations. The magnetic properties of the spin ferromagnetic Ising model on MnAs compound using the high-temperature series expansions of magnetic susceptibility are investigated. As a result, The Néel temperature $T_C(K)$ is estimated from the divergence of the magnetic susceptibility with an exponent. All values are comparable with those reported in [29, 30] and fit with the universality hypothesis [31].

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