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First-Principles Materials Study for Spintronics: MnAs and MnN

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We report *ab-initio* all electrons density- functional calculations for the electronic structure of the compounds MnAs and MnN, in the zinc-blende phase. They are potential materials for use in fabrication of new functional semiconductors taking advantage of the spin degree of freedom. The aim is the establishing of the semiconductor spin electronics (spintronics) as a practical technology [H. Ohno, Semiconductor Science and Technology **17**, 4 (2002).]. We compare results obtained using the theoretical approaches LDA (Local Density Approximation) and GGA (Generalized Gradient Approximation). The calculations are spin-polarized and we follow the evolution of the band structures as a function of lattice parameter. We compare also the evolution of the density of states of the majority-spins and of the minority-spins. We conclude that, depending on the lattice parameter, both materials may be half-metallic, therefore showing conduction by charge carriers of one spin direction exclusively: the majority- spin band is continuous, while the minority-spin has a gap. Both materials reach a total magnetization of the order of $4 \mu_B$. MnN changes from paramagnetic to ferromagnetic with the increase of the lattice parameter.

1 Introduction

The Mn atom as a constituent of the so called diluted magnetic semiconductors (DMS) is nowadays the object of many experimental and theoretical investigations [1-12]. In the present work we compare the electronic and magnetic properties of MnAs and MnN in the hypothetical zinc-blende (ZB) phase. Although the ZB is not the ground-state structure for these materials [13-19], we find interesting to study them in the ZB structure, since in it the Mn atoms find the same local environment as in diluted alloys, such as $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ or $\text{Ga}_{1-x}\text{Mn}_x\text{N}$ ($x < 0.07$). The tetrahedral coordination of the Mn atoms seems to play an important role in the understanding of the properties of the III-V DMS. Therefore, we study the compounds MnAs and MnN in the ZB structure in order to have a better understanding of the nature of the chemical bond of Mn tetrahedrally coordinated with As or N in the III-V DMS.

2 Theoretical framework

We carry out first-principles band structure and total-energy calculations within the framework of the density functional theory [20] and compare the results for two approaches, namely the local density approximation (LDA) and the generalized gradient approximation (GGA). We use the full-potential linearized-augmented plane-wave method as implemented in the Wien2k code [21] and applied to a 2-atoms unit cell. The muffin-tin radii adopted were 2.0 a. u. (Mn), 1.89 a. u. (As) for MnAs and 1.75 a. u. (Mn), 1.44 a.u. (N) for MnN. The Rkmax parameter was taken as 8.0 and

the angular momentum $l=10$ for the expansions inside the spheres. The total energy and eigenvalues were converged to 10^{-5}eV , and 10^{-4}eV , respectively. The calculations were performed with spin-polarized potentials in order to analyze the ferromagnetic phases of the compounds. We follow the behavior of the band structures, density of states, fermi level, and magnetic moments as a function of the lattice parameter.

3 Results and discussion

In Fig. 1 we show the behavior of the cell magnetic moment as a function of lattice parameter. One can see that the magnetic moments for MnN are zero at the equilibrium lattice parameters ($a_o = 4.19 \text{ \AA}$ (LDA), and 4.30 \AA (GGA)); for MnAs the magnetic moments are $2.5\mu_B$ and $4.0\mu_B$ respectively at the equilibrium lattice parameters $a_o = 5.32 \text{ \AA}$ (LDA) and 5.71 \AA (GGA). It is noticeable that the magnetization undergoes large changes induced by small changes in the lattice parameters. The LDA values always tend to be lower than the GGA ones. In both approaches it is predicted that expansions (compressions) tend to turn the materials more ferromagnetic (paramagnetic). In the case of MnN the ferromagnetic phase should appear at moderate expansions over the equilibrium lattice parameter. This behavior should be understandable by looking at the band structures and density of states. We note that the magnetic coupling between the Mn atom and the As atom or N atom is always antiferromagnetic. It can be seen in Fig. 1 that the magnetic moments increase as the lattice parameters increase and tend to saturate at the value $4.0 \mu_B$ in both cases. The saturation of the magnetization at the value $\sim 4.0 \mu_B$

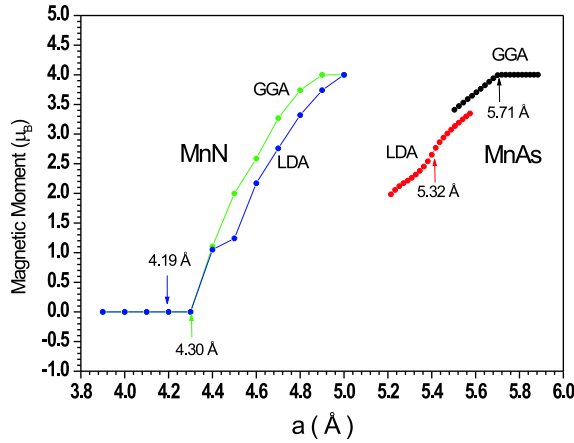


Figure 1. Magnetization, per unit cell, for the compounds MnN and MnAs as a function of the lattice parameter in both approaches LDA and GGA. The arrows indicate the equilibrium lattice parameters.

may be understood on the basis of a model of charge transfer from Mn to the neighbors' 4p (As) and 2p (N) shells [10]. This charge transfer is not complete due to the strong interaction originating from the p-d hybridization. As the unit cell is expanded this hybridization is reduced and the Mn atom tends to a configuration with four valence electrons which, following Hund's rule, reaches a magnetic moment of $4.0 \mu_B$. On the other hand this p-d interaction leads to quite large negative polarization of the anions ($\sim -0.10 \mu_B$), being larger for As than for N. As the lattice parameters increase the spin polarization turns to be effective and this is reflected in the electronic band structures and density of states. In Fig. 2 we show the band structures and density of states for MnN and MnAs, both at the equilibrium lattice parameter and calculated in the GGA approach. The band structures exhibit the levels originated from atomic states Γ_1 (N-2s, As-4s), Γ_{15p} (N-2p, As-4p), Γ_{12} (Mn-3d) and Γ_{15d} (Mn-3d), at the Γ point. In the case of MnN, the N-2p valence band appears as the first Γ_{15p} level, below the Fermi level, E_F , for both minority-spin and majority-spin systems. The Γ_{12} bands originated from N-3d states are entirely occupied, while the Γ_{15d} bands are empty. On the other hand, in the case of MnAs the minority-spin and majority-spin systems have different band structures. For the minority-spin system the low lying Γ_{15p} band is As-4p in origin, and the Γ_{12} and Γ_{15d} bands are empty. For the majority-spin system the low lying Γ_{15d} band is Mn-3d in origin, the Γ_{12} band is occupied and the Γ_{15p} band is half-filled.

Detailed calculations show that as the unit cells evolve from compressed geometries to expanded geometries the calculated band structures change differently depending on the spin-polarization. For the MnN compound the LDA and GGA calculations carried out by taking the lattice parameter varying from $a=4.10 \text{ \AA}$ to $a=5.00 \text{ \AA}$ exhibit the same qualitative behavior. The majority-spin bands evolve from a situation in which the Fermi level is exactly on the edge of a fully occupied Γ_{12} band to a situation in which the Fermi level cuts through the higher lying Γ_{15d} band, which turns to be partially occupied; at the same time the minority-spin bands evolve to a situation in which the Fermi level

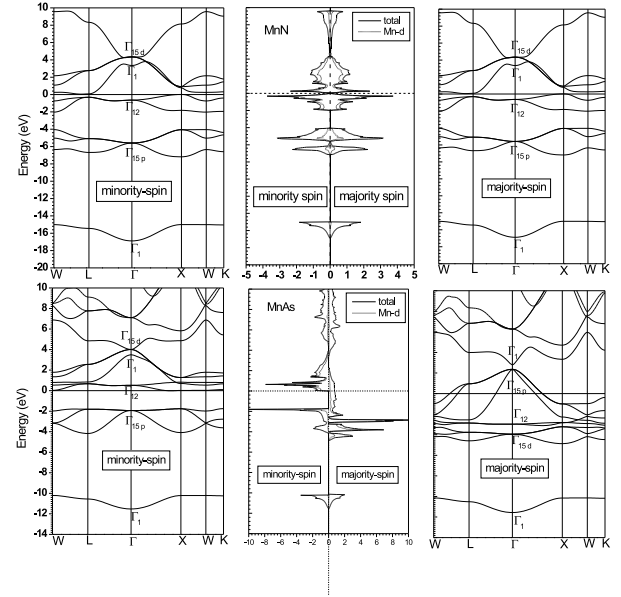


Figure 2. Electronic structures for zinc-blende MnN (top) and MnAs (bottom) at the GGA total energy minimum ($a_0=4.30 \text{ \AA}$ -MnN and $a_0=5.71 \text{ \AA}$ -MnAs). The figures on the left and on the right correspond to the band structures for the minority-spin and majority-spin, respectively. The figures in the middle correspond to the density of states. The horizontal line refers to the position of the Fermi level.

just touch an empty Γ_{12} band, being on the edge of the big gap between Γ_{15p} and Γ_{12} . Therefore in this range of lattice parameters the MnN material changes from a paramagnetic metallic phase to a ferromagnetic phase in which the majority-spin system is metallic and the minority-spin is isolating. With regard to the MnAs compound both LDA and GGA calculations also give qualitative similar results. As long as the lattice parameter is varied from $a=4.80 \text{ \AA}$ to 5.90 \AA the majority-spin system keeps a metallic character with the Fermi level lying successively higher across the Γ_{15p} band; meanwhile the minority-spin system evolves from a metallic character in which the Fermi level lies in the middle of the Γ_{12} band to an isolating character in which the Fermi level lies in the gap between the Γ_{15p} and Γ_{12} bands.

4 Conclusion

Based on our first-principles calculations we conclude that both materials, MnN and MnAs, may be half-metallic in zinc-blende stretched lattices in which $a_0 > 4.90 \text{ \AA}$ for MnN and $a_0 > 5.71 \text{ \AA}$ for MnAs, therefore showing conduction by charge carriers of one spin direction exclusively. The majority-spin band is continuous, while the minority-spin has a gap. Both materials reach a total magnetization of the order of $4 \mu_B$. MnN changes from paramagnetic to ferromagnetic with the increase of the lattice parameter.

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