Journal of Magnetism and Magnetic Materials 385 (2015) 27–31

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

First-principles calculation on dilute magnetic alloys in zinc blend crystal structure

Hamid Ullah [a,*], Kalsoom Inayat [a], S.A .Khan [b], S. Mohammad [b], A. Ali [c], Z.A. Alahmed [d], A.H. Reshak [e,f]

[a] Department of Physics, Government Post Graduate Jahanzeb College, Saidu Sharif Swat, Pakistan
[b] Department of Physics, Materials Modeling Laboratory, Hazara University, Mansehra 21300, Pakistan
[c] Department of Advanced Materials Science & Engineering, Hanseo University, Seosan-si, Chungnam-do 356-706, Republic of Korea
[d] Department of Physics and Astronomy, King Saud University, Riyadh 11451, Saudi Arabia
[e] New Technologies-Research Center, University of West Bohemia, Univerzitni 8, 306 14 Pilsen, Czech Republic
[f] Center of Excellence Geopolymer and Green Technology, School of Material Engineering, University Malaysia Perlis, 01007 Kangar, Perlis, Malaysia

ARTICLE INFO

Article history:
Received 26 November 2014
Received in revised form
10 February 2015
Accepted 27 February 2015
Available online 2 March 2015

Keywords:
Dilute magnetic semiconductor
Spintronic
Half metalicity
Density of states

ABSTRACT

Ab-initio calculations are performed to investigate the structural, electronic and magnetic properties of spin-polarized diluted magnetic alloys in zinc blende structure. The first-principles study is carried out on Mn doped III–V semiconductors. The calculated band structures, electronic properties and magnetic properties of $Ga_{1-x}Mn_xX$ (X=P, As) compounds reveal that $Ga_{0.75}Mn_{0.25}P$ is half metallic turned to be metallic with increasing x to 0.5 and 0.75, whereas substitute P by As cause to maintain the half-metallicity nature in both of $Ga_{0.75}Mn_{0.25}As$ and $Ga_{0.5}Mn_{0.5}As$ and tune $Ga_{0.25}Mn_{0.75}As$ to be metallic.

Calculated total magnetic moments and the robustness of half-metallicity of $Ga_{0.75}Mn_{0.25}P$, $Ga_{0.75}Mn_{0.25}As$ and $Ga_{0.5}Mn_{0.5}As$ with respect to the variation in lattice parameters are also discussed. The predicted theoretical evidence shows that some Mn-doped III–V semiconductors can be effectively used in spintronic devices.

1. Introduction

The III–V semiconductors and their alloys are extensively used in photonics and optoelectronics. These materials are mostly used for high-frequency light emitting diodes, optical detectors and laser diodes due to their high melting points, high thermal conductivity, large bulk modulus and wide band gaps. The binary compounds GaP and GaAS have been very promising candidates for advance technology. Most interestingly their band gap can be varied by alloying. This alloying effectively increases the range of applications of GaP and GaAs compounds [1–7].

Diluted magnetic semiconductors (DMS) are very promising materials for optoelectronic and spintronics applications. III–V compounds when doped with 3d transition elements this turn them to be as III–V DMS. The III–V DMS compounds attracted consideration for the possible increase in efficiency and miniaturization of the electronic devices [16]. Different DMS compounds [7–15] have been intensively studied theoretically as well as experimentally to design efficient devices like super smart diodes, super smart memory chips, spin valves and spin field effect transistors. It is essential to explain the known properties of a given material designed for the fabrication of highly efficient electronic and spintronics devices and even to predict different properties of hypothetical materials.

For the analysis and calculation, computer modeling and simulation techniques are used as a consequence of the complication in the growth, characterization and procedure of these properties. The prediction of different properties of materials has been simplified by the use of modern technology and computational techniques with the first principle calculation. The computational techniques have already been applied to numerous materials with the first principle and predicted that theoretical results agree well with the experimental results.

In this article the structural, electronic and magnetic properties of $Ga_{1-x}Mn_xP$ and $Ga_{1-x}Mn_xAs$ (x=0.25, 0.50, 0.75) alloys are studied by using density functional theory (DFT) within the state-of-the-art all-electron full potential linear augmented plane wave (FPLAPW) method as implemented in WIEN2k code [17], which has proven to be one of the most accurate methods for the computation of the electronic structure of solids within DFT [18–21]. The ground state energy, optimum volume, bulk modulus, derivatives of the bulk modulus, band structures and density of states

* Corresponding author.
E-mail address: hamidullah@yahoo.com (H. Ullah).

http://dx.doi.org/10.1016/j.jmmm.2015.02.069
0304-8853/

are calculated and analyzed in details. The magnetic properties are predicted through the density of states analysis and magnetic moments.

2. Method of calculation

In the full-potential scheme, radial function, times waves function, potential and charge density are extended into two basis sets. Inside each atomic sphere the wave function is extended in spherical harmonics while in interstitial region it is extended to plane-wave basis. In similarly fashion the potential is extended as [22,23].

$$V(r) = \begin{cases} \sum_{lm} V_{lm}(r) Y_{lm}(\hat{r}) \end{cases} \quad (1a)$$

$$V(r) = \begin{cases} \sum_{K} V_K e^{iKr} \end{cases} \quad (1b)$$

Here Eq.1a is express the potential inside the sphere, whereas Eq.1b for the potential in the interstitial site. Inside the sphere the wave function is extended in terms of spherical harmonics up to $l_{max}=9$. The potential is constant outside the sphere while spherically symmetric within the muffin-tin sphere. For the transition metal doped with III–V semiconductors the plane wave cut-off value of $K_{max}*R_{MT}$ is chosen to be equal to 8. On the basis of convergence test, a mesh of 120 **k**-points and $G_{max}=24$ are used for well converged results.

3. Results and discussions

3.1. Structural properties

To calculate the ground state properties of $Ga_{0.75}Mn_{0.25}X$, $Ga_{0.50}Mn_{0.50}X$ and $Ga_{0.25}Mn_{0.75}X$ (X=P, As), the volume of super cell was optimized by Birch Murnaghan's equation of state [23]. The optimization is also important to expose the magnetic nature of the alloys. The total energy as function of volume of the alloys is calculated for ferromagnetic and anti-ferromagnetic states. The total energy difference ($\Delta E = E_{AFM} - E_{FM}$) as listed in Table 1 show that the ferromagnetic states are more stable than that of anti-ferromagnetic states. The other structural parameters are also mentioned in the Table 1. At the optimized volume we have calculated the structural parameters such like the lattice constant a, bulk modulus B and derivative of the bulk modulus B^P within general gradient approximation (PBE-GGA) as shown in Table 1. Following Table 1, it is obvious that by increasing the concentration of Mn in GaP and GaAs the lattice constant decreases due to the smaller volume of Mn than Ga. Similarly by substituting P by As the lattice constant also decreases due to the smaller volume of As than P. The spin polarized electronic band structures, magnetic properties and robustness of half-metallicity are further calculated by using the calculated lattice constants.

Table 1
Calculated lattice constant a_0, Bulk Modulus B, Derivative of Bulk Modulus, B^P, and ground state ferromagnetic (FM) and anti-ferromagnetic (AFM) energies $Ga_{0.75}Mn_{0.25}X$, $Ga_{0.50}Mn_{0.50}X$ and $Ga_{0.25}Mn_{0.75}X$ (X=P, As).

Parameters	$Ga_{0.75}Mn_{0.25}$P/As	$Ga_{0.50}Mn_{0.50}$P/As	$Ga_{0.25}Mn_{0.75}$P/As
Lattice constant (Å)	5.49/5.69	5.45/ 5.73	5.42/5.71
Bulk modulus (GPa)	80.25/76.98	67.76/53.03	82.64/67.58
B^P	5.0/5.0	5.0/5.0	5.0/5.0
E_{FM} (Ry)	−16718.973818/ −32063.406665	−7566.529118/ −15249.934951	−13576.980958/ −28921.700885
E_{AFM} (Ry)	−16718.973814/ −32063.406663	−7566.529116/ −15249.934948	−13576.980954/ −28921.700882

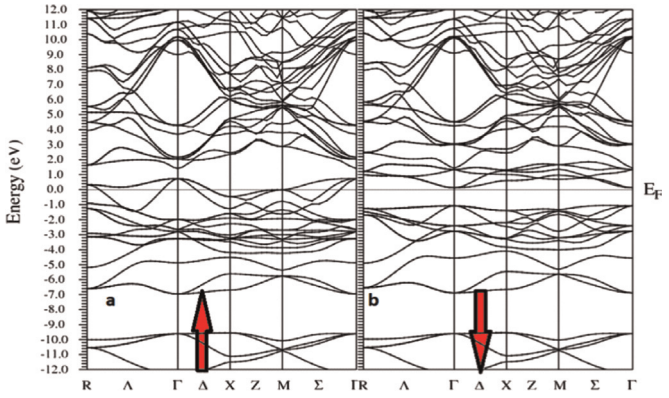

Fig. 1. Calculated band structure of $Ga_{0.75}Mn_{0.25}P$. (a) Spin (↑) and (b) Spin (↓).

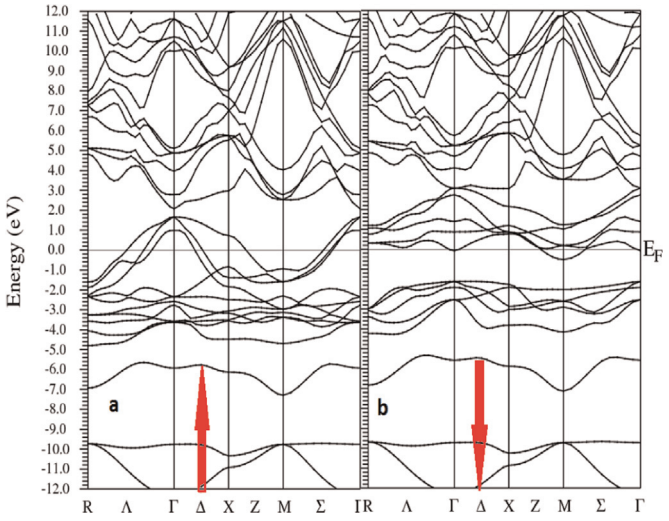

Fig. 2. Calculated band structure of $Ga_{0.50}Mn_{0.50}P$. (a) Spin (↑) and (b) Spin (↓).

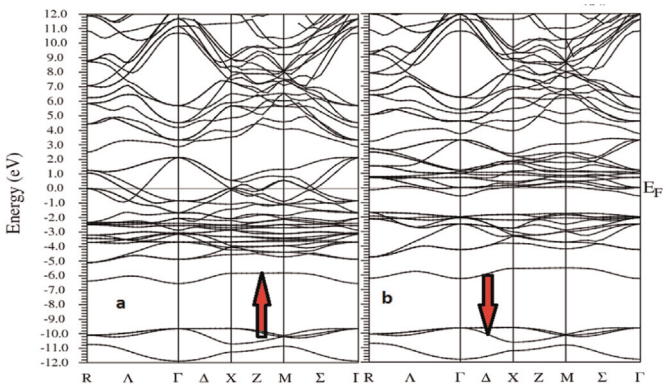

Fig. 3. Calculated band structure of $Ga_{0.25}Mn_{0.75}P$. (a) Spin (↑) and (b) Spin (↓).

3.2. Band structure and density of states

The spin polarized electronic band structures in the first Brillouin zone are calculated along the symmetry directions for $Ga_{0.75}Mn_{0.25}X$, $Ga_{0.50}Mn_{0.50}X$ and $Ga_{0.25}Mn_{0.75}X$ (X=P, As), as prototype we show the electronic band structures of $Ga_{1-x}Mn_xP$