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Ab Initio Study of Structural and Electronic Properties of GaP and $Ga_{0.875}Fe_{0.125}P$ using First Principle Calculations

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ABSTRACT

We investigated the structural and electronic Properties of GaP and $Ga_{0.875}Fe_{0.125}P$ diluted Magnetic Semiconductor in Zinc Blende (B3) phase. The calculations have been performed using Density functional theory as implemented in the Spanish Initiative for Electronic Simulations with Thousands of Atoms code using local density approximation as exchange-correlation (XC) potential. The calculated spin polarized energy band structures show that $Ga_{0.875}Fe_{0.125}P$ is metallic in nature for both spin up and spin down states. Calculated results are also compared with available previous theoretical and experimental.

I. INTRODUCTION

Modern technology of spintronics i.e. spin based electronics is based on the spin of charge carriers and play wonderful role in emerging field of new multi-functional devices [1-5]. The semiconductors formed from elements of groups III and V have important properties and have important place in semiconductor industry. Due to this, the study of these materials and ternary alloys of such materials i.e. dilute magnetic semiconductors (DMS) attracts a lot of attention of researchers in experimental as well as theoretical field. [6-8]. Doping of transition metal atoms in GaP has been under research due to its interesting properties that may contribute in the development of spintronic appliances [9-17].

II. COMPUTATIONAL METHOD

In our research paper, we have studied structural and electronic properties of pure GaP and $Ga_{0.875}Fe_{0.125}P$ using Density Functional Theory as implemented in SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) code [18]. We have used Local Density Approximation (LDA) parameterized by CA as exchange correlation potential [19]. The structural parameters including Lattice constants within the range of experimental values, mesh cut-off are optimized to the equilibrium total energy. Using 2×1×1 dimension standard sixteen atoms per supercell and substituting the Gallium atom at (0, 0, 0) position with Fe atom, constructed the crystal structures of $Ga_{0.875}Fe_{0.125}P$ under discussion. Including semi-core Fe-3d states as valence electrons in our calculations, we have generated norm-conserving pseudopotentials in the manner of Troullier and Martins [20]. An energy shift of 80 meV and Double zeta polarization (DZP) basis set is used for these spin polarized calculations.

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III. RESULT AND DISCUSSION

3.1. Structural Properties

In this paper, we have studied the zinc blende structure of GaP and $Ga_{0.875}Fe_{0.125}P$. We investigated the total energy values for several values of lattice constants in the range of lattice constant of pure GaP [21]. For structural optimization Murnaghan's equation [22] of state is used by minimizing the total energy with respect to unit cell volume. Figure 1 represents the structural optimization for GaP and $Ga_{0.875}Fe_{0.125}P$ compounds and these optimized lattice parameters are further used to study the detailed analysis of electronic properties of compounds under discussion. On replacement of one Ga atom with Fe metal atom, we observe a small decrement in lattice constant value. This is explained on the basis that atomic size of Fe is less than the Ga because of increased nuclear attraction for valence electrons in case of Fe.

3.2. Electronic Properties:

Calculated spin polarized energy band structures along with TDOS of pure GaP and $Ga_{0.875}Fe_{0.125}P$ are shown in Fig. 2 and Fig. 3 respectively. The detailed analysis of these structures show that on doping of Fe atom in GaP semiconductor, basic properties of GaP have been significantly modified. For complete description of the atomic and orbital origin of different bands, we have calculated the partial DOS of Ga, P, and Fe atoms as shown in Fig. 4. Even though, fundamental properties of pure GaP are already well calculated, but we have explored spin polarized band structure along with TDOS and partial DOS of Ga and P in Fig. 3 and 4 respectively to compare the various electronic states of Fe impurity atom.

The energy band structure of $Ga_{0.875}Fe_{0.125}P$ reveals that top of valence band maximum crosses the Fermi energy level for the majority spin state. For minority spin state, valence band maximum remain below the fermi level but, bottom of conduction band minimum crosses the Fermi energy level. Hence, $Ga_{0.875}Fe_{0.125}P$ is metallic for both spin states. The new states have been generated at Fermi level E_F, which accounts for magnetism on replacement of Ga atom with Fe atom. The tetrahedral crystal field of surrounding P atoms split the five fold degenerate energy shells of 3d orbitals of Fe atom into two energy levels i.e. twofold degenerate e_g (d_z^2 and $d_{x^2-y^2}$) having lower energy content and three-fold degenerate t_{2g} (d_{xy}, d_{xz}, d_{yz}) having high energy content. The detailed study of PDOS of $Ga_{0.875}Fe_{0.125}P$ compound represents that the DOS in lower parts of valence band from mainly arises due to Ga-4s, 4p states and P-3s states for both majority spin states and minority spin states. The states above these states are Fe-3d and P-3p states. In case of $Ga_{0.875}Fe_{0.125}P$, P-3p and Fe-3d states undergo hybridization near the Fermi energy level and mainly contribute to the top of valence band and bottom of the conduction band. Due to hybridization between these states, valence band maximum and conduction band minimum cross the Fermi energy level in majority spin channel and minority spin channel respectively and show metallic behavior. The differentiation between spin up and spin down states is mainly due to the hybridization of the Fe-3d and P-3p states.The nature of attraction in DMS can be explained by spd exchange splitting. For spin up and spin down states, the spd exchange splitting is calculated by the band-edge spin splitting of the conduction band minima and valence band maxima at Γ symmetry point [23-25] as

$\Delta E_C = E_{CBM}^{\downarrow} - E_{CBM}^{\uparrow}$ and $\Delta E_V = E_{VBM}^{\downarrow} - E_{VBM}^{\uparrow}$

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Where, $E_{CBM}^{\downarrow}$ is conduction band minimum of spin down state, $E_{CBM}^{\uparrow}$ is conduction band minimum of spin up state,

$E_{VBM}^{\downarrow}$ is valence band maximum of spin down state and $E_{VBM}^{\uparrow}$ is valence band maximum of spin up state

The calculated band gap parameters and exchange splitting parameters are given in Table 1.We have also studied the detailed partial densities of states of Fe-3d, Fe-3d (t2g) and Fe-3d(eg) of $Ga_{0.875}Fe_{0.125}P$ under our discussion and are shown in Fig. 5.

Table 1. Calculated lattice constants, Spin down band gap $\Delta E_g^{\downarrow}$, Spin up Band gap $\Delta E_g^{\uparrow}$, Valence band edge splitting (ΔE_C), Conduction band edge splitting (ΔE_V) and other parameters of GaP and $Ga_{0.875}Fe_{0.125}P$.

Compound/ Property	LC (Å)	B (GPa)	$\Delta E_g^{\downarrow}$	$\Delta E_g^{\uparrow}$	$E_{CBM}^{\downarrow}$	$E_{CBM}^{\uparrow}$	$E_{VBM}^{\downarrow}$	$E_{VBM}^{\uparrow}$	ΔE_C	ΔE_V
GaP	5.63 5.516[a] 5.45[b]	80.90 76.51[a] 88.00[c]		0.859		0.4327		-0.4196		
$Ga_{0.875}Fe_{0.125}P$	5.56		0.5769	0.9970	-0.1196	1.2282	-0.6963	0.2312	-1.3478	-0.9277

[a] Ref. [26], [b] Ref. [27], [c] Ref. [28]

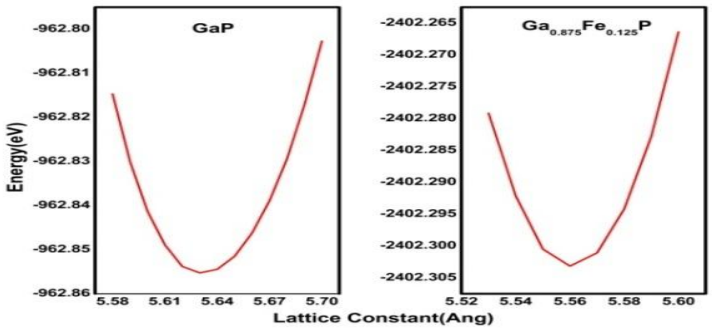

Fig 1. The structural optimization for GaP and $Ga_{0.875}Fe_{0.125}P$.

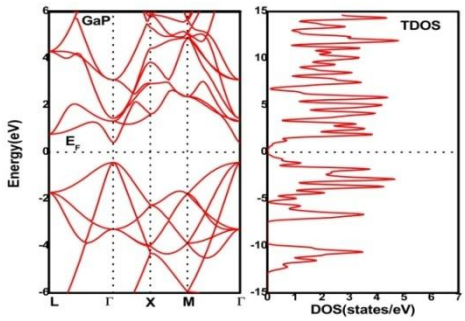

Fig 2. Band Structure and TDOS of GaP.

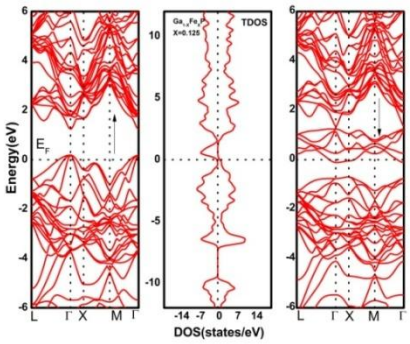

Fig 3. Spin-polarised Band Structures and TDOS for spin up and spin down of $Ga_{0.875}Fe_{0.125}P$.

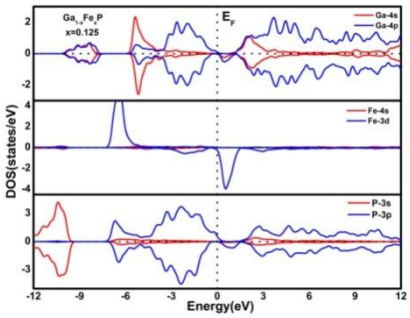

Fig 4. Calculated Partial Density of states of $Ga_{0.875}Fe_{0.125}P$.

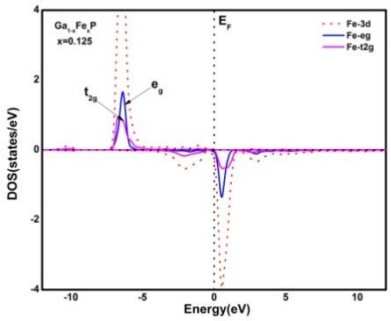

Fig 5. Projected density of states (PDOS) of Fe-3d, Fe-t_{2g} and Fe-e_g of $Ga_{0.875}Fe_{0.125}P$.

IV. CONCLUSION

In the present work, we have calculated the structural and electronic properties of pure GaP and $Ga_{0.875}Fe_{0.125}P$ in zinc blende phase by first principle DFT calculations using Local density Approximation (LDA) parameterized by CA as exchange correlation. We investigated that in case of $Ga_{0.875}Fe_{0.125}P$, P-3p and Fe-3d states undergo hybridization near the Fermi energy level and due to hybridization between these states, valence band maximum and conduction band minimum cross the Fermi energy level in majority spin channel and

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minority spin channel respectively and show metallic behavior. Calculated results are in good agreement with previous theoretical and experimental studies.

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