Generating magnetic response and half-metallicity in GaP via dilute Ti-doping for spintronic applications

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ABSTRACT

Existence of band gap in one spin channel and metallic character in other leads to interesting magnetic and optical properties of any material. These materials are capable to generate fully spin polarized current and are responsible for maximizing the efficiency of spintronic devices. The present work explores the electronic and magnetic properties of Ti-doped GaP compound with dopant concentrations; $x = 0.02$, 0.03 and 0.06 in order to search new Diluted Magnetic Semiconductor (DMS) compounds as spintronic materials using full potential linearized augmented plane wave plus local orbitals (FPLAPW + lo) method. The generalized gradient approximation (GGA) is used to decide exact exchange-correlation (XC) potentials. The calculated results showed that the total magnetic moment of ~1.00 μ_B gets induced after Ti-doping in GaP at all dopant concentrations, irrespective of any magnetic element present. Further, this doping also generates half-metallicity in GaP with a half-metallic (HM) gap at Fermi level (E_F) in minority spin channel. The half metallicity is originated by the hybridization of Ti-d states with P−p states. This induced magnetism appeared in the systems is the result of exchange interactions between host (GaP) and Ti-atom.

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1. Introduction

Right from the discovery of half metallicity in semi Heusler alloy by de Groot et al. [1], a lot of attentions were paid to analyze the electronic and magnetic properties of different types materials in order to search new half-metallic ferromagnets [2−10]. Among these materials, DMSs are the most promising materials for the spintronic devices as these can be characterized as true half metallic ferromagnets with 100% spin polarization at Fermi level (E_F) after suitable doping with appropriate atom. Moreover, the substitution of 3d transition metals (TMs) on semiconductors becomes prominent, owing to the possibility of combining magnetism and semiconducting properties [11,12]. The researchers showed interests rigorously in DMS compounds after Munekata

et al. [13] synthesized Mn-doped InAs by low temperature-molecular beam epitaxy (LT-MBE) technique. Active experimental research on DMS compounds was initiated in last decade of 20th century using molecular beam epitaxy (MBE) and laser ablation [3,14] methods.

Initially, Ohno et al. [3,14,15] successfully discovered the ferromagnetism in $Ga_{1-x}Mn_xAs$ (x = 1−10%) compounds using LT-MBE technique and boosted the attention of the researchers into III−V based DMSs. After that a lot of efforts were made for the synthesis of ferromagnetic semiconductors in the past decades [2−5]. In the last few years, the research on TM doped III−V DMSs have been extended in order to predict the high Curie temperature (T_C), improved ferromagnetic properties and to explore the mechanism behind the half metallic ferromagnetism (HMF) [10,16−19]. In the category of III−V semiconductors, GaP is an important material which characterizes in cubic Zinc Blende (ZB) structure and can be used in wide variety of electronic equipments such as optoelectronic devices, cellular phones and semiconductors lasers etc.

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GaP is considered as a suitable host material to make DMS compounds after doping with TMs as justified by the some theoretical and experimental reports [10,20–25]. The optical absorption and photoluminescence spectra of Ti-doped GaP measured at various magnetic field values at T = 2 K by Halliday et al. [20]. They observed the Zeeman splitting of the sharp line spectra. The evidence of ferromagnetism with higher T_C ~ 600 K was reported by Owens [21] in GaP doped with 3% Mn using ferromagnetic resonance (FMR) and AC magnetization measurements. Owens synthesized the sample by bulk sintering process and claimed that this room temperature ferromagnetism arises in the sample due to the dilute distribution of Mn^{2+}. Two years later, Owens et al. [22] observed the room temperature ferromagnetism in bulk sample of Cu-doped GaP up to doping concentration, $x = 0.03$ using simple solid state reaction method. They also performed the total energy calculations using the Projector Augmented Wave (PAW) method and reproduced their experimental findings. Gosk et al. [23] found the superconducting behavior with critical temperature, 6.2 K in Cr-doped GaP and GaAs crystals by the liquid encapsulated Czochralski (LEC) method.

The *ab-initio* electronic structure calculations of some III–V, II–VI based DMS compounds were performed by Yoshida and Sato [24] using Korringa Kohn Rostoker-Coherent Potential Approximation (KKR-CPA) method within mean field approximation (MFA). They observed that out of studied compounds, Mn-doped AlP, GaP and InP with 5% dopant concentration exhibit room temperature ferromagnetism. A systematic investigation of electronic and magnetic properties of 3d transition metal doped GaP and GaAs compounds were carried out by Zhi et al. [25] using Vienna ab initio simulation package (VASP). They concluded that V-, Cr- and Mn-doped GaP and GaAs compounds at doping concentration of 25% show room temperature ferromagnetism and are most promising materials for spintronic applications. Saini et al. [10] analyzed the electronic and magnetic properties of Cr-doped GaP for various Cr concentrations ($x = 0.03, 0.0625, 0.125$ and 0.25) using full-potential linearized augmented plane-wave plus local orbitals (FPLAPW + lo) method. They showed that the half metallicity remain intact as dopant concentration is reduced to dilute limit (<0.1).

The origin of magnetism in semiconductors containing non-magnetic atoms was analyzed by the various research groups [16,18]. Recently, electronic and magnetic properties of Ti-doped AlP at various dopant concentrations, $x = 0.03, 0.0625, 0.125$ and 0.25 were studied by Liang et al. [18] using both density functional theory (DFT) and DFT + U approaches. They observed that Zener's double exchange mechanism and p-d hybridization are responsible for half-metallic ferromagnetism and also estimated the Curie temperature higher than 599 K.

The experimental synthesis of Ti-doped GaP [20] motivated us to check the magnetic response and half-metallicity on theoretical front using DFT approach. Further, the solubility limit of TMs in III–V based DMS compounds is < 8–10% [26]. Thus, this limit for Ti doping in GaP should be preferred as < 8% for producing authentic data and to verify experimental findings. With this aim, we have calculated the electronic and magnetic properties of Ti-doped GaP for doping concentrations $x = 0.02, 0.03$ and 0.06. The other aim of present investigation is to check the variation of half-metallicity on reducing the dilute limit.

2. Theoretical approach

The electronic structure calculations of Ti-doped GaP DMS compound were carried out using the highly precise all electrons FPLAPW + lo method based on DFT [27] as implemented in WIEN2k code [28]. The exchange and correlation (XC) potentials were constructed using the generalized gradient approximation (GGA) within the parameterization of Perdew-Burke-Ernzerhof (PBE) [29]. In FPLAPW + lo calculations, the core states were treated fully relativistically while valence states and semi-core states were treated semi-relativistically (i.e. ignoring the spin orbit coupling). The plane wave cut off parameters were decided by $R_{MT}k_{max} = 8$ (where k_{max} is the largest wave vector of the basis set such that k_{max} controls the accuracy of the calculation). The Fourier expansion of potential in the interstitial region was expanded up to $G_{max} = 14$ a.u.$^{-1}$ and the maximum value of partial waves inside the atomic sphere was $l_{max} = 10$. The calculations were based on the supercell approach where one Ga atom at (0,0,0) in the supercell of GaP is replaced by Ti-atom. The supercells of $(2 \times 2 \times 3)$, $(2 \times 2 \times 2)$ and $(2 \times 2 \times 1)$ with 96, 64 and 32 atoms have been constructed to achieve ~ 2%, 3% and 6% doping, respectively. The non-overlapping muffin-tin radii (R_{MT}) of Ga, Ti and P were chosen as large as possible so as to obtain nearly touching spheres and to ensure minimize interstitial space. The energy convergence criterion was set to 10^{-4} Ry and the charge convergences were also monitored along with it. The k-space was carried out using the modified tetrahedron method [30] with 8, 10 and 50 k-points in the irreducible Brillouin zone (IBZ) for doping of 2.08%, 3.125% and 6.25%, respectively.

3. Results and discussion

It is important to excess suitable lattice parameters for Ti-doped GaP. To cater this need, the lattice parameters were optimized for each doping concentrations in the neighborhood of experimental lattice parameters of host GaP [31] in ferromagnetic configurations which are listed in Table 1. These optimized parameters were used further to find ground state properties of studied semiconducting compounds.

In order to check the structural stability of the Ti-doped GaP DMS compound at all dopant concentrations $x = 0.02, 0.03$ and 0.06 the formation energies were calculated using the expression:

$$E_{for} = E_{cell} - E_{base}^0 - xE_{dopant}^0 + xE_{Ga}^0$$

where E_{cell}, E_{base}^0, E_{dopant}^0 and E_{Ga}^0 are the total energy of Ti-doped GaP, host GaP, dopant Ti and Ga, respectively, and x is dopant concentration. The computed formation energies for all doping concentrations; $x = 0.02, 0.03$ and 0.06 are -207.77 Ry, -311.21 Ry and -622.36 Ry, respectively, shows the stability of these compounds in the ZB structure. Moreover, it also shows that resultant DMS compounds are most stable at $x = 0.06$.

The total density of states (TDOS) of the studied compounds at all dopant concentrations, shown in Fig. 1 reveal that the energy gap appearing in the minority spin channel, due to the splitting of

Table 1
Optimized lattice parameters (a), energy gap (E_g) and HM gap (E_{HM}) in minority spin channel, total and atom resolved magnetic moments of $Ga_{1-x}Ti_xP$ ($x = 0.02, 0.03,$ and 0.06) DMS compounds. M_{int} represents magnetic moment found in the interstitial region.

	$Ga_{1-x}Cr_xP$		
	x = 0.02	x = 0.03	x = 0.06
a (Å)	5.528	5.527	5.519
E_g (eV)	1.572	1.550	1.370
E_{HM} (eV)	0.580	0.547	0.301
M_{tot} (μ_B)	1.002	1.012	0.999
M_{Ti} (μ_B)	0.690	0.697	0.686
M_{Ga} (μ_B)	0.015	0.018	0.020
M_P (μ_B)	−0.011	−0.010	−0.015
M_{int} (μ_B)	0.299	0.298	0.301

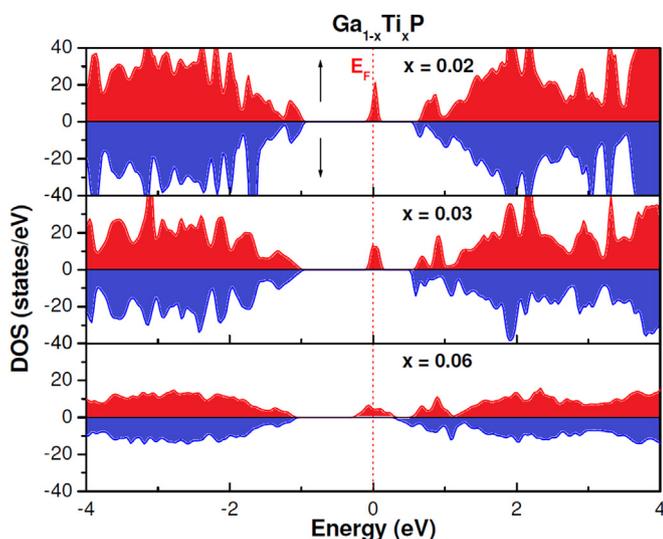**Fig. 1.** Calculated total DOS of $Ga_{1-x}Ti_xP$ ($x = 0.02, 0.03$ and 0.06) DMS compounds.

DOS at E_F leads to 100% spin polarization. The pure GaP is good semiconductor with a band gap of 2.32 eV [31], but its properties get changed drastically when it is doped with Ti-atom. We observed an appreciable band gap (E_g) > 1.5 eV in minority spin channel for each doping in GaP as listed in Table 1. The metallic behavior in majority and semiconducting in minority spin channel governs the resultant DMSs as true half metallic ferromagnets. This type of materials can be characterized as true half-metallic ferromagnets. Due to the existence of this peculiar behavior, these compounds are able to generate fully spin polarized current and are responsible for maximizing the efficiency of spintronic devices. Moreover, the existence of HM gap i.e. a minimal gap for spin excitation in minority spin channel is a striking feature of studied DMS compounds and it should be calculated for the clear understanding of half metallicity in these compounds. This gap is defined as the minimum value out of ($E_F - E_v^{top}$) or ($E_c^{bot.} - E_F$), where E_v^{top} and $E_c^{bot.}$ represent the energy corresponding to top of VB and bottom of CB, respectively. In other words, a true HM farromagnet is governed by a non zero HM gap instead of band gap in any spin
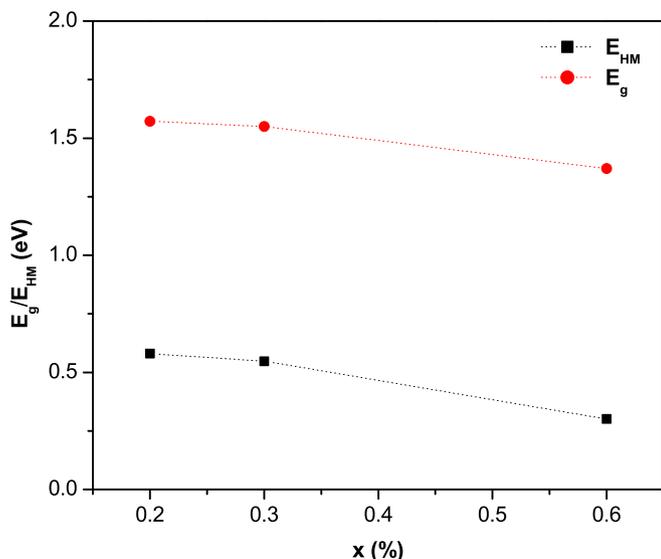
channel [32,33]. The HM gap (E_{HM}) decreases as we move towards the non-solubility limit (Table 1 and Fig. 2). This is due to the localized nature of Ti-d states at E_F whose extent decreases on increasing the dopant concentration from $x = 0.02$ to 0.06. The Ti-d states hybridized strongly with P−p states at lowest doping level ($x = 0.02$), resulting in a gap for minority spin channel with largest spacing between bonding (e_g) and antibonding (t_{2g}) states.

In order to analyze the contribution of various states (responsible for the half metallic behavior of these compounds) in the vicinity of E_F, the spin dependent partial DOS (PDOS) of $Ga_{1-x}Ti_xP$ ($x = 0.02, 0.03$ and 0.06) compounds, are shown in Fig. 3. The DOS from −4.0 eV to −1.0 eV are mostly attributed to Ti-d and P−p states with relatively small contribution of Ga-p states for the both spin channels. In the majority spin, the states at E_F exhibit a mixed character of Ti-d states with P−p states which are most important to induce magnetism in these compounds. On the other hand, as we visualize carefully the top of valence band (VB) and bottom of the conduction band (CB) in minority spin channels the Ti-d and P−p states play a major role to decide a band gap at E_F, whereas the share from Ga-s, Ga-p and P-s states to the total DOS are almost negligible for both spin channels.

The appearance of HM ferromagnetism in this compound can be explained in the framework of theory of crystal filled splitting in which the P-ions splits the Ti-3d states into a three fold degenerate t_{2g} (d_{xy}, d_{zx}, d_{yz}) and a doubly degenerate e_g (d_z^2, d_{x-y}^{22}) states. The hybridization of these non bonding orbital containing T-e_g states and P−p states and antibonding orbitals, formed by Ti-e_g states and P−p states, plays a crucial role to decide the ferromagnetism in the resultant DMS compounds at all dopant concentrations (x). Due to the strong p-d hybridization, the partially filled Ti-t_{2g} antibonding states forms in the gap and lowers the total energy to stabilize a ferromagnetic ground state and also accountable for the separation of the two symmetry states in the minority spin channel and to induce an HM gap. This type of behavior can be explained by using the Zener's p-d exchange model [34,35] and double exchange mechanism [36] as well. Therefore, we claim that these mechanisms attribute the different electrons densities for majority and minority electrons and thus are responsible for the emergence of ferromagnetism in the studied systems. This type of behavior is in support of other theoretical prediction as proposed by Liang et al. [18] for Ti-doped AlP.

The calculated total magnetic moment per unit cell (M_{tot}) and atom resolved spin magnetic moments of Ti-doped GaP at all dopant concentrations, are listed in Table 1. The calculated total magnetic moment per unit cell (M_{tot}) is ~1.00 μ_B for all dopant concentrations although there is no magnetic ion in this system. When the tetravalent Ti-atom is substituted in place of a trivalent Ga atom, three electrons are donated to make a bond with P atoms and remaining one electron occupies the impurity bands at E_F which generates the magnetic state in resultant DMS compounds. Clearly, the Ti-atom contributes to total magnetic moment (~0.70 μ_B) significantly and remains stationary for all dopant concentrations. But, the induced moment on Ga-/P-atom is negligibly small, which align parallel/antiparallel to Ti-atom, respectively. These results suggest that the induced magnetism is due to the exchange interaction between host and Ti-atoms. It is also important to emphasize here that electron−phonon interaction also influences the behavior of spin currents and play a significant role to decide the spintronic effect observed [37].

The ground state valence charge densities of undoped GaP in the plane (110) have been analyzed in Fig. 4, in order to check the status of chemical bonding between the atoms. For undoped GaP, the charge density is spread out more around P atom than Ga atom due to the extra valence electrons with P, whereas Ga atom has more core electrons populated near the nucleus. Due to the
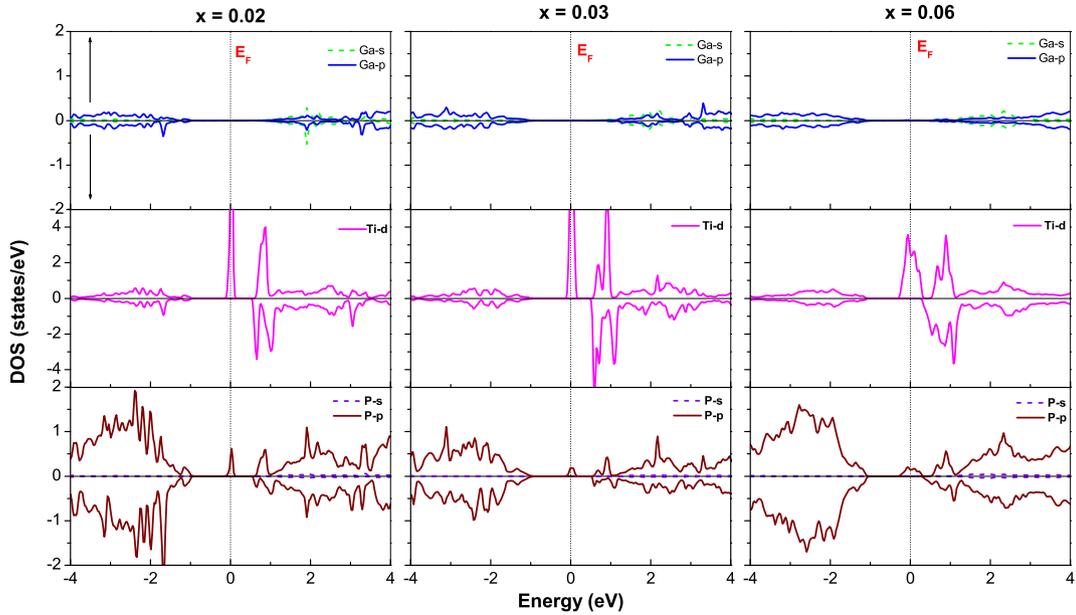

Fig. 2. Variation of band gap and HM gap in minority spin channel of $Ga_{1-x}Ti_xP$ ($x = 0.2, 0.3$ and 0.06) DMS compounds.

Fig. 3. Calculated atom resolved DOS of $Ga_{1-x}Ti_xP$ (x = 0.02, 0.03 and 0.06) DMS compounds.
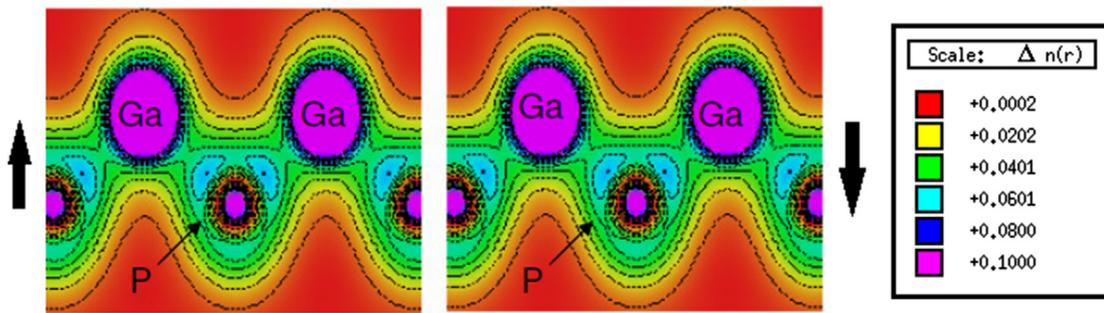

Fig. 4. Spin polarized charge density plots of pure GaP semiconductor in (110) plane.

electronegativity difference between Ga and P-atoms, the charge transfer takes place from Ga to P, which governs the polar covalent nature of GaP compound.

The bonding nature of the resultant compounds modify drastically as shown in Fig. 5(a), (b) and (c), as we introduce dopant Ti-atom into GaP. The characteristics of Ga−P and Ti−P bonds vary with dopant concentration. The contour plots of charge density indicate the accumulations of charge along the Ti−P bonds and show the tendency of ionic character of the bonds depending on Pauling electro-negativity difference of the atoms. The charge
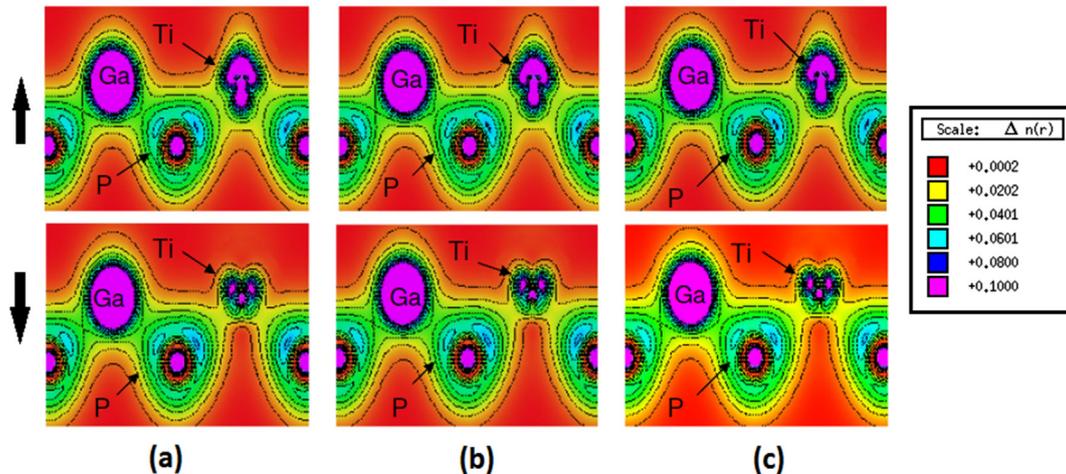

Fig. 5. Spin polarized valence charge density plots of Ti-doped GaP DMS compounds with dopant concentrations as (a) x = 0.02 (b) x = 0.03 (c) x = 0.06 in (110) plane in the units of e/a.u.^{3}.

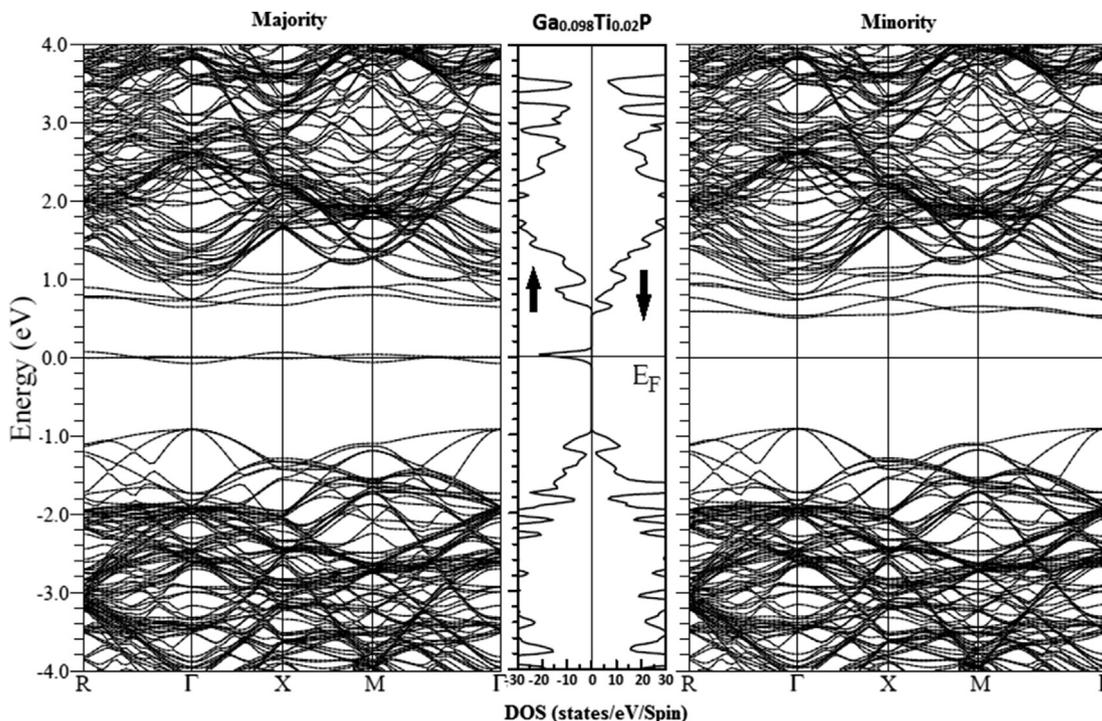**Fig. 6.** Spin resolved band structure and total DOS of $Ga_{0.98}Ti_{0.02}P$. The horizontal line at E = 0 eV marks the Fermi level (E_F). We set the zero-point of energy (Fermi level) at the valence band maximum (VBM).

density is more in the Ga–P bond than Ti–P bond, which shows the strong overlap and governs the more covalent character. The electrons population is greater in the majority spin case than that in the minority spin for all dopant concentrations due to the presence of partially occupied $Ti-t_{2g}$ states at E_F.

The spin polarized band structure of $Ga_{0.98}Ti_{0.02}P$ ($x = 0.02$) with TDOS along the high symmetry directions of the first Brillouin zone is presented as a reference for all studied compound in Fig. 6, in order to examine the nature of the bands at and near E_F. It is clear that due to the substitution of Ti-atom in GaP, the resultant DMS compound exhibits half metallic character with 100% spins polarization at E_F. In majority spin channel, the band at E_F is contributed significantly by the overlapping of $Cr-t_{2g}$ and $Cr-e_g$ states with a small admixture of P–p states and governs the metallic character for this spin. But in minority spin band, no such states are present at E_F resulting semiconducting band gap for minority spin. This band gap is found to be direct along Γ- Γ direction which enhances the potential of resultant DMS in optoelectronic devices with an advantage of spin transport. The next empty bands at bottom of CB are overwhelming dominant by $Ti-t_{2g}$ followed by $Ti-e_g$ states.

4. Summary and conclusions

A full potential treatment of electronic and magnetic properties of non-magnetic Ti-doped GaP at dopant concentrations; $x = 0.02$, 0.03 and 0.06 is presented with in the solubility limit. We observed that the dopant introduces band gap in minority spin channel and metallic character in majority spin channel at all studied dopant concentrations and the resultant DMS are characterized as true half metallic ferromagnets. This band gap and HM gap in minority spin channel decreases as we move towards the non-solubility limit. The half metallicity is originated by the hybridization of Ti-d states with P–p states. The contour plots of charge density indicate that the characteristics of Ga–P and Ti–P bonds vary with dopant concentration.

The total magnetic moment per unit cell (M_{tot}) of 1.00 μ_B has been found in the studied DMS for all dopant concentrations. The Ti-atom is the main contributor to the total magnetic moment and the induced moment on Ga and P atoms are negligibly small which aligns parallel and antiparallel to Ti-atom, respectively. The induced magnetism is due to the exchange interaction between host (GaP) and Ti atom. Due to the existence of this peculiar behavior, these compounds may be potential candidates in manufacturing spintronic devices.

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