Cr-doped GaP DMS compound
Chapter 3

3.1 Introduction

The III-V semiconductors are the very imperative type of semiconductors belonging to III and V group of periodic table. They are already used in wide variety of electronic equipment in the form of electronic and optoelectronic devices, including cellular phones (microwave transistors), compact disks (semiconductor lasers), and in many other applications. Therefore, the introduction of magnetic III-V semiconductors opens up the possibility of using a variety of magnetic phenomena not present in conventional nonmagnetic III-V semiconductors in the optical and electrical devices already established. When III-V semiconductor doped with some magnetic elements such as Mn, their properties get changed significantly from the conventional nonmagnetic III-V semiconductor. These materials are the one of the most suited candidates for spintronic materials after appropriate doping with some elements because these are the ideal materials for fabricating all spin based semiconductor devices. But, the major obstacle in making III-V semiconductors as magnetic is the low solubility of magnetic elements in the host semiconductor [1-3]. Actually, the stability of these materials within the solubility limit is the great challenge to both, experimentalist and theorist. A considerable breakthrough came into the picture in 1990s by using MBE technique and laser ablation [4-12], a thin-film growth technique in vacuum. These methods were capable to introduce doping concentration beyond thermal equilibrium solubility limit such that the actual solubility limit could be achieved.

A lot of efforts have been made for the synthesis of ferromagnetic semiconductors in the past decades [4-14]. First of all, Ohno et al. [7-9] successfully developed new Mn doped GaAs and InAs ferromagnetic semiconductors with doing concentration, x = 1-10 % using LT-MBE technique. The discovery of ferromagnetism in (Ga,Mn)As with $T_c = 110^\circ$ K, boosted the attention of the researchers into III-V based DMSs. Recently, research on III-V
based DMSs have been extended towards materials containing magnetic elements other than Mn in order to predict the improved ferromagnetic properties and to explore the mechanism behind the half metallic ferromagnetism (HMF) [3,15-18]. The Cr-doped III-V semiconductors in zinc blende structure are the promising DMS materials on which considerable efforts have been employed in order to find out the HMF, spin polarization and high $T_C$ [17-20]. A thin films of Cr-doped GaAs with doping concentration, $x = 0.10$ were grown by Saito et al. [21] using LT-MBE method and studied the magnetic and transport properties. Abe et al. [22] prepared the GaSb films with small dopant concentration of Cr by MBE method and showed that this compound exhibits ferromagnetic behaviour at room temperature. Recently, a systematic study of magnetic circular dichroism (MCD) has been carried out for a series of $(\text{Ga}_{1-x},\text{Cr}_x)\text{As}$ epilayers with $x = 2.38$ and $4.59\%$ by Wu et al. [23] using LT-MBE technique and established the ferromagnetism by superconductor quantum interference device (SQUID) measurements. The first principle calculations of electronic structure of some III-V based DMS compounds were investigated by Saito et al. [24] using Korringa Kohn-Rostoker-Coherent Potential Approximation (KKR-CPA) method within mean field approximation (MFA). They observed that out of studied compounds, Cr-doped GaN and GaAs exhibit room temperature ferromagnetism.

Gallium Phasphide (GaP) is one of the indirect band gap materials of the III-V series in zinc blende phase. Its ternary transition metal (TM) compounds such as TM-doped GaP can offer the advantage that such devices can be operated for large number of applications at room temperature. In this contrast, a bulk sample of Cu-doped GaP was successfully grown by Owens et al. [25] using simple solid state reaction method and observed room temperature ferromagnetism up to doping concentration, $x = 0.03$. They also performed the total energy calculations using the Projector Augmented Wave (PAW) method and reproduced the same experimental findings. Gosk et al. [26] cultivated the bulk GaP and GaAs crystals with high Cr concentration by the liquid encapsulated Czochralski...
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(LEC) method and found superconducting behaviour with critical temperature, 6.2°K for both compounds.

Several ab-initio calculations have been reported to understand the magnetic properties in TM-doped GaP. Schulthess et al. [27] employed the self interaction corrected local spin density (SIC-LSD) method to compute the electronic and magnetic properties of some Mn-doped III–V based DMS compounds and predicted the proper electronic ground state configuration for Mn in GaAs, GaP, and GaN. A systematic investigation of electronic and magnetic properties of 3d transition metal doped GaP and GaAs compounds have been carried out by Zhi et al. [28] using Vienna ab-initio simulation package (VASP). They concluded that V-, Cr- and Mn-doped GaP and GaAs compounds at x = 25% show room temperature ferromagnetism and are most promising materials for spintronic applications. Recently, Huang et al. [29] analyzed the structural, electronic and magnetic properties of Cr-doped GaP for various Cr concentrations (x = 0.125, 0.25, 0.50 and 0.75) using FPLAPW method within GGA as XC potential. These compounds were found to be half metallic and the HM character is maintained up to the compression in lattice constant by 7.8, 5.7 and 4.2% of its actual value for doping concentration, x = 0.125, 0.25 and 0.50, respectively, in this study.

The magnetism in TM-doped GaP has been studied extensively. However, the Cr-doped GaP based DMS compound has not been well studied theoretically within the solubility limit (< 8-10 %). An expansive supercell calculation is needed for predicting the ground state properties of this DMS compound. The stable HMF at lower doping concentration is great challenge to the theoreticians. Therefore, an emphasis is to be conferred on the study with concentration x ≤ 0.125 for exhaustive comparison with experiments in future. Hence, keeping in mind the dilute limit of TMs in this compound, we have calculated the electronic and magnetic properties of Cr-doped GaP at four Cr-concentrations, x = 0.25, 0.125, 0.06 and 0.03. The efforts have been made to search the new DMS
compounds and to understand the origin of magnetism with the help of spin polarized DOS, band structure. Moreover, the other aim of present study is to check the retainness of half metallicity on decreasing dopant concentration.

3.2 Details of the calculations

The first principle calculations of Ga\textsubscript{1-x}Cr\textsubscript{x}P DMS compound were carried out using the FPLAPW method based on density functional theory (DFT) [30] as implemented in WIEN2k code [31]. The XC potential has been constructed using GGA within the parameterization of Perdew-Burke-Ernzerhof (PBE) [32]. In FPLAPW calculations, the core states are treated fully relativistically where as for the valence states, a semirelativistic calculation is performed. The plane wave cut off parameters were decided by $R_{MT}k_{max} = 7$ (where $k_{max}$ is the largest wave vector of the basis set such that $k_{max}$ controls the accuracy of the calculation) and $G_{max} = 14$ a.u.$^{-1}$ for Fourier expansion of potential in the interstitial region. The radius of MT spheres ($R_{MT}$) for Ga, Cr and P atom were chosen to be 2.1, 2.0, and 1.6 a.u., respectively, ensuring nearly touching spheres and minimizing the 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 integration has been carried out using the modified tetrahedron method [33] with 150, 40, 30 and 10 $k$-points in the irreducible Brillouin zone (IBZ) for doping of 25 %, 12.5 %, 6.25 % and 3.125 %, respectively.

The GaP compound is crystallizes in zincblende (ZB) structure with space group $216(F\bar{4}3m)$. The coordinates for Ga atom is chosen to be (0,0,0) and for P atom is chosen to be (1/4,1/4,1/4) as shown in Fig. 3.1. The figure also shows the corresponding Brillouin zone (BZ) and its irreducible wedge (IBZ). To construct the electronic structure for Ga\textsubscript{1-x}Cr\textsubscript{x}P at $x = 0.25/0.03$, a suitable supercell ($1\times1\times1)/(2\times2\times2)$ of GaP consisting of 8/64 atoms is selected and in this cell, one Ga-atom at origin is replaced by Cr atom.
Fig. 3.1  Unit cell (left side) and BZ, with its IBZ, for ZB crystal structure of GaP. The symmetry k-points are shown on IBZ.

Fig. 3.2  (1×1×1) Supercell for crystal structure of Ga$_{1-x}$Cr$_x$P at x = 0.25.

The corresponding supercell for doping 25%/3% is depicted in Fig. 3.2/3.3. Heavy computational resources are needed to find out the ground state for 3 % doping as the supercell (2×2×2) of 64 atoms. On the other hand, a tetragonal (2×1×1)/(2×2×1) supercell has been generated with 16/32 atoms is generated to ensure 12.5 %/6.25 % Cr-doping in GaP, shown in Fig. 3.4/3.5. Again, one Ga-atom at origin is replaced by Cr-atom to simulate the desired doping in this cell.
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Fig. 3.3  (2×2×2) Supercell for crystal structure of Ga$_{1-x}$Cr$_x$P at $x = 0.03$.

Fig. 3.4  (2×1×1) Supercell for crystal structure of Ga$_{1-x}$Cr$_x$P at $x = 0.125$.  

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Fig. 3.5 (2×2×1) Supercell for crystal structure of Ga$_{1-x}$Cr$_x$P at x = 0.06.

3.3 Results and discussion

We have summarized from the literature, some important ground state properties in Table 3.1 for the overview of experimental studies performed for GaP compound which is used as host material to construct DMS compound by Cr-doping.

Table 3.1: List of experimental crystallographic and ground state properties of GaP compound.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Experimental Crystal structure</th>
<th>Ground state</th>
<th>Experimental band gap (eV)</th>
<th>Characterization techniques</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaP</td>
<td>B3</td>
<td>Semiconducting</td>
<td>2.35</td>
<td>Photoelectron emission spectroscopy, Photoelectrochemical</td>
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<tr>
<td></td>
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<td>Water splitting</td>
</tr>
</tbody>
</table>
3.3.1 Ground state properties

The structural optimization for Ga$_{1-x}$Cr$_x$P compounds with $x = 0.25$, 0.125, 0.06 and 0.03 as depicted in Fig. 3.6, has been performed in the neighborhood of lattice parameters of parent GaP semiconductor [34]. The equilibrium values of optimized lattice parameters are listed in Table 3.1. These parameters have been used to carry out the detailed analysis of electronic and magnetic properties of studied DMS compound. A small increment in lattice constants is observed on decreasing the dopant concentration.

![Graph showing total energy versus lattice parameters of Ga$_{1-x}$Cr$_x$P DMS compound](image)

**Fig. 3.6** Total energy versus lattice parameters of Ga$_{1-x}$Cr$_x$P DMS compound with $x = 0.25$, 0.125, 0.06 and 0.03. The solid lines show a polynomial fit for determining the optimized lattice constants. $E_{\text{equi}}$ corresponds to equilibrium energy at optimized lattice constant.
The optimized lattice parameters for $x = 0.125$ and 0.25 are in accordance with previous prediction [29] where as for $x = 0.03$ and 0.06, the same are reported for the first time. The values of the HM gap ($E_{HM}$ (eV)) in MIC, spin and total magnetic moments at Cr, Ga and P sites as well as total magnetic moment for the compound at $x = 0.25$, 0.125, 0.06 and 0.03 from this work and other [29] are reported in Table 3.1.

Table 3.1: Optimized lattice parameters, the HM gap ($E_{HM}$ (eV)) in MIC, total and atom resolved magnetic moments of $\text{Ga}_{1-x}\text{Cr}_x\text{P}$ ($x = 0.25$, 0.125, 0.06 and 0.03) DMS compound. Here $M_{\text{int}}$ represents magnetic moment at interstitial site.

<table>
<thead>
<tr>
<th></th>
<th>Ga$_{1-x}$Cr$_x$P</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$(Å)</td>
<td>$x = 0.25$</td>
</tr>
<tr>
<td></td>
<td>$x = 0.125$</td>
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<tr>
<td></td>
<td>$x = 0.06$</td>
</tr>
<tr>
<td></td>
<td>$x = 0.03$</td>
</tr>
<tr>
<td>$E_{HM}$ (eV)</td>
<td>5.501, 5.435$^a$</td>
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<tr>
<td></td>
<td>5.512, 5.439$^a$</td>
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<td></td>
<td>5.517</td>
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<tr>
<td></td>
<td>5.523</td>
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<tr>
<td>$M_{\text{tot}}$ $(\mu_B)$</td>
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<tr>
<td></td>
<td>0.451, 0.470$^a$</td>
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<td></td>
<td>0.712</td>
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<tr>
<td></td>
<td>0.720</td>
</tr>
<tr>
<td>$M_{\text{Cr}}$ $(\mu_B)$</td>
<td>3.002, 3.000$^a$</td>
</tr>
<tr>
<td></td>
<td>3.012, 3.000$^a$</td>
</tr>
<tr>
<td></td>
<td>3.003</td>
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<tr>
<td></td>
<td>3.009</td>
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<tr>
<td>$M_{\text{Ga}}$ $(\mu_B)$</td>
<td>2.847, 2.761$^a$</td>
</tr>
<tr>
<td></td>
<td>2.856, 2.735$^a$</td>
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<td>2.851</td>
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<tr>
<td></td>
<td>2.861</td>
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<tr>
<td>$M_{\text{P}}$ $(\mu_B)$</td>
<td>0.028, 0.031$^a$</td>
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<tr>
<td></td>
<td>0.012, 0.018$^a$</td>
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<td></td>
<td>0.005</td>
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<tr>
<td></td>
<td>0.002</td>
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<tr>
<td>$M_{\text{int}}$ $(\mu_B)$</td>
<td>-0.065, -0.054$^a$</td>
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<tr>
<td></td>
<td>-0.034, 0.049$^a$</td>
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<td>-0.022</td>
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<tr>
<td></td>
<td>-0.016</td>
</tr>
<tr>
<td>$M_{\text{int}}$ $(\mu_B)$</td>
<td>0.329</td>
</tr>
<tr>
<td></td>
<td>0.341</td>
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<tr>
<td></td>
<td>0.343</td>
</tr>
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<td></td>
<td>0.341</td>
</tr>
</tbody>
</table>

Ref. [29]

3.3.1.1 Density of states (DOS)

The total DOS (TDOS) of the studied compounds is presented in Fig. 3.7. The energy gap appearing in the minority spin channel (MIC) due to the splitting of DOS at $E_F$ leads to 100% spin polarization at all concentrations. Moreover, the existence of HM gap i.e. a minimal gap for spin excitation in MIC is a striking feature of studied DMS compound. This gap is of unique importance for creating a
hole and an electron in MIC. It is defined as the minimum value out of \((E_F - E_{v\text{top}}})\) or \((E_{c\text{bot}} - E_F)\), where \(E_{v\text{top}}\) and \(E_{c\text{bot}}\) represent the energy corresponding to top of VB and bottom of CB, respectively. A true HM ferromagnet is governed by a non zero HM gap instead of band gap in any spin channel [35,36]. Thus, it is to be calculated for clear understanding of half metallicity in the compound. All these compounds are able to generate fully spin polarized current due to feasible spin excitation and are responsible for maximizing the efficiency of spintronic devices. The values of HM gaps at various dopant concentrations are presented in Fig. 3.8, which show that this gap increases on decreasing the doping concentration (x) from 0.25 to 0.03.

![Fig. 3.7](image)

**Fig. 3.7** Calculated total DOS of Ga\(_{1-x}\)Cr\(_x\)P DMS compound (x = 0.25, 0.125, 0.06 and 0.03).
This behaviour is attributed to the localized nature of Cr-d states whose extent increases on decreasing the dopant concentration from $x = 0.25$ to 0.03. Therefore, at lowest doping, Cr-d states hybridized strongly with P-p states resulting in a gap in the MIC with largest spacing between bonding and antibonding states. Our calculated HM gap for $x = 0.25$ and 0.125 supports corresponding value calculated by Huang et al. [29] using same methodology as mentioned in Table 3.1.

![Graph](image)

**Fig. 3.8** Variation of HM gap of $\text{Ga}_{1-x}\text{Cr}_x\text{P}$ with the doping concentrations, $x = 0.25, 0.125, 0.06$ and 0.03.

The partial contributions towards total DOS in studied compound at various dopant concentrations are almost alike for same dopant. Thus, we have explored the spin dependent PDOS of $\text{Ga}_{1-x}\text{Cr}_x\text{P} \ (x = 0.03)$ compound only as a
The detailed investigation of PDOS reveals that the DOS in valence band (VB) from \(-7.0\) eV to \(-4.7\) eV originates mainly from Ga-s states with an admixture of P-p states for both spin channels. The DOS from \(-4.7\) eV to \(-1.0\) eV are mostly attributed to the Cr-d and P-p states with relatively small contribution of Ga-p states for the both spin. In the majority spin, the states at \(E_F\) exhibit a mixed character of Cr-d states with P-p states which are most important to induce HM ferromagnetism in these compounds. The bottom of the conduction band (CB) is mainly contributed by the Cr-d states in MIC only, whereas the Ga-s, p and P-p states contribute equally for both spin channels.

**Fig. 3.9** Calculated total and partial DOS of \(\text{Ga}_{1-x}\text{Cr}_x\text{P}\) \((x = 0.03)\) compound. Spin polarized TDOS of GaP semiconductor is shown for exhaustive evaluation.
In order to show the importance of Cr-d states, we have also plotted the spin polarized DOS of host GaP semiconductor in the uppermost panel of Fig. 3.9. The TDOS in Ga$_{1-x}$Cr$_x$P ($x = 0.03$) DMS compound have different shape in the vicinity of $E_F$ for MAC and MIC due to hybridization of Cr-d states with P-p states, whereas the corresponding TDOS is identical for both spin channels in host GaP. In GaP semiconductor, the s,p-states of Ga and P are filled up to $E_F$ whereas in Cr-doped GaP compound, these are shifted deeper in the VB for MIC. On the other hand, a non bonding orbital comprising of Cr-$e_g$ states and P-p states and antibonding orbital consisting of Cr-$t_{2g}$ states and P-p states are present due to hybridization which governs the HM character of this compound. The actual band gap of GaP is 2.32 eV [34] but we observe a smaller band gap (1.57 eV) in MIC for Ga$_{1-x}$Cr$_x$P ($x = 0.03$) DMS compound. It is due to the fact that although the VB gets shifted towards lower energy from $E_F$ but the CB exhibits more shifting toward $E_F$ due to the presence of less energetic antibonding states originating from hybridization of Cr-d and P-p states in MIC. This reduces the gap from actual semiconducting gap.

3.3.1.2 Bandstructure

The spin resolved band structure of Ga$_{1-x}$Cr$_x$P ($x = 0.03$) as a reference compound along the high symmetry directions of the first Brillouin zone is presented in Fig. 3.10. The band gap is direct along $\Gamma$- $\Gamma$ direction. The band structures of Ga$_{0.97}$Cr$_{0.03}$P in both, MAC and MIC indicate that the low lying bands at $\sim$ -4.7 eV to $\sim$ -1.0 eV arises due to Cr-d and P-p states with a small admixture of Ga-p states. In MAC, the next band is contributed significantly by the overlapping Cr-$t_{2g}$ and Cr-$e_g$ states with a small admixture of P-p states. This band is pushed in the vicinity of $E_F$ by the exchange splitting and governs the metallic nature. But in MIC, no such band is present at $E_F$ which confirms the semiconducting nature of this compound. The next empty bands at bottom of CB are also overwhelming dominant by Cr-$t_{2g}$ followed by Cr-$e_g$ states.
3.3.1.3 Magnetic Properties

It is well clear now that the magnetic properties of these compounds depend on the dopant concentrations and on the valence electron concentration. The total magnetic moment per unit cell (\(M_{\text{tot}}\)) and atom resolved spin magnetic moments calculated at optimized lattice parameters for present compounds are listed in Table 3.1. When a Cr atom (with six valence electrons) is substituted in place of a trivalent Ga atom, three electrons are donated to make a bond with P atoms and remaining electrons occupy the impurity bands at \(E_F\) which generates the magnetic state in resultant DMS compounds. The half metallic behavior of this compound is consistent with the integral value of magnetic moment of the unit cell, i.e. 3 \(\mu_B\). The similar magnetic moment at all concentrations is a characteristic of localized
magnetic moment on Cr-impurity. As the host, Ga and P atom are non magnetic and the magnetic moment at these atoms in resultant DMS compounds is of induced character from Cr-atom. As a consequence, only Cr-atom contributes to total magnetic moment moment which remains stationary at all concentrations. The induced moment on Ga and P atoms is negligibly small which aligns parallel and antiparallel to Cr-atom, respectively. Hence Ga/P interacts ferromagnetically/antiferromagnetically with Cr atom. This induced magnetic moment decreases at both, Ga and P atoms on reducing the dopant concentration from 0.25 to 0.03 because lesser Cr-d states are available at lower concentration for p-d hybridization.

3.3.1.3.1 Origin of Magnetism

In order to stabilize the magnetism (ferromagnetism or anti-ferromagnetism) in magnetic materials, the identification of correct exchange mechanism is very important. For DMSs, in which the doping concentrations is very small, the physical understanding of the exchange mechanisms involved is still doubtful, since no simple and straightforward magnetic interaction exists. Thus, a multitude of mechanisms can lead to ferromagnetism or anti-ferromagnetism and some of them might even act simultaneously. The relevant exchange mechanisms that dominate the magnetic properties of DMSs are Zener’s double exchange [37-40], Zener’s p–d exchange [41-45] and superexchange mechanism [46,47].

In the present case, the stabilization of the ferromagnetism in all Ga$_{1-x}$Cr$_x$P compounds owes to the Zener’s double-exchange mechanism as the Fermi level falls within the partially occupied majority band of 3d impurity states. Sato et al. [48,49] also discussed the ferromagnetic mechanism in various DMS compounds in the similar way. However, for a quick understanding of this mechanism, a brief theme is outlined as under:
This mechanism predicts the relative ease with which an electron may be exchanged between two species and has important implications for whether materials are ferromagnetic, antiferromagnetic, or nonmagnetic. Further this, mechanism is a type of a magnetic exchange that may arise between ions present in different oxidation states only.

The Cr-d states play a crucial role to decide the ferromagnetism and HM gap induced in the resultant DMS compound at various dopant concentrations (x). The comparison of d-DOS of Cr-atom at various value of x is explored in Fig. 3.10. A small/large DOS in CB for MAC/MIC leads to almost fully/empty d-states in VB/CB. The Cr-d states are most localized at $E_F$ for lowest doping concentration, $x = 0.03$. With a decrease in dopant concentration from $x = 0.25$ to $0.03$, the broadening of impurity band decreases which leads to localization of higher order and become responsible for enlarging the HM gap as stated earlier. Due to the tetrahedral environment of P atoms, the five fold degenerate atomic levels of Cr-d states get splitted into a two fold degenerate $e_g$-state ($d_{z^2}, d_{x^2-y^2}$) and a threefold degenerate $t_{2g}$-state ($d_{xy}, d_{xz}, d_{yz}$), resulting in formation of bonding and antibonding states.

![Fig. 3.11](Image)

Calculated d-DOS of Cr atom in Ga$_{1-x}$Cr$_x$P ($x = 0.25, 0.125, 0.06$ and $0.03$) compound.
A strong p-d exchange interaction in Cr-d and P-p is accountable for separation of these two symmetry states in MIC. This p-d hybridization in the compound leads to the double exchange mechanism. Consequently, this mechanism attributes the different electrons densities for majority and minority electrons and thus is responsible for emergence of ferromagnetism in this system.

3.4 Conclusions

To summarize, we have presented first principle prediction of electronic and magnetic properties of Cr-doped GaP at dopant concentration, \( x = 0.25, 0.125, 0.06 \) and 0.03 to search new candidates showing HM ferromagnetism. We predict, using FPLAPW method, that this compound is half metallic ferromagnets at all dopant concentrations. The most exciting characteristics of this compound is that the half metallicity remains intact on reducing the solubility limit of Cr atom with an enhanced HM gap at \( E_F \) in MIC for smallest dopant concentration (\( x = 0.03 \)). This property makes this compound suitable for practical spintronic devices and favors the need of growing it experimentally. The d-states of impurity atom (Cr) play a crucial role to induce the magnetism in the studied compound. The interaction between Cr-d states and P-p states pushes the symmetric d-states at \( E_F \) in MAC and away from \( E_F \) in MIC which originates a gap in the latter at all dopant concentrations. These Cr-d states are most localized at \( E_F \) for lowest doping concentration, \( x = 0.03 \) results a large HM gap for that concentration. The double exchange mechanism is responsible for emergence of ferromagnetism in this system. The HM character of this compound is consistent with the integral value of magnetic moment of the unit cell. We have also observed that the magnetic properties of this compound depend on the dopant concentrations and on its valence electron configuration. The main contribution in the total magnetic moment comes from Cr-d states. As the host, Ga and P atom are non magnetic and the magnetic moment at these atoms in resultant DMS compounds is negligibly small and of induced character from Cr-atom. The p-d interaction between Cr and
P atoms reduces the magnetic moment of Cr atom from its elemental value and induces small local spin magnetic moment on nonmagnetic Ga/P atom which aligns parallel/antiparallel to Cr atom. This induced magnetic moment decreases at both, Ga and P atoms on reducing the dopant concentration from 0.25 to 0.03 because lesser Cr-d states are available at lower concentration for p-d hybridization.
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