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INFLUENCE OF EXCHANGE AND CORRELATION INTERACTIONS ON THE SPIN POLARIZED ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF $Ga_{0.75}Mn_{0.25}P$ IN THE B3 ZINC BLENDE STRUCTURE

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This study focuses on investigating the influence of exchange and correlation interactions on the spin polarized electronic structure and magnetic properties of $Ga_{0.75}Mn_{0.25}P$ in the B3 Zinc Blende phase. First-principle calculations were performed by systematically varying the Hartree-Fock (HF) exchange (α) value from 0 to 25% using the onsite exact-exchange functional for the treatment of the correlated electrons. The electronic and magnetic properties unveil that $Ga_{0.75}Mn_{0.25}P$ manifests a half-metallic ferromagnetic behaviour at deferent values of HF exchange. Moreover, as the fraction (α) parameter increases, the band gap increases, leading to modifications in the spin polarized band structures. Additionally, our investigations indicate that exchange and correlation interactions cause an increase in the lattice parameter and volume of the compound. Furthermore, these interactions result in a decrease in the magnetic moments of P and Ga atoms, while the Mn moments increase. These findings provide valuable insights into the behavior of $Ga_{0.75}Mn_{0.25}P$ and offer potential applications in the design of spintronic devices.
Keywords: *HF Exchange; Correlated electrons; GaMnP; Magnetic material; Half-metallic; Spintronic*
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INTRODUCTION

Diluted Magnetic Semiconductors (DMS) and spintronics (spin-based electronics) are two fascinating fields of research in semiconductor physics that intersect through the study of materials like III-V (GaX, InX, AlX……. X= As, P, N….) or II-VI (CdX, ZnX, MgX……. X = S, Se, Te….) doped with magnetic ions having a 3d layer or a 4f layer of transition metals or rare earths (lanthanides). These materials have gained considerable interest for their potential in spintronics applications.

Spintronics seeks to exploit the charge and spin of electrons for the development of new functionalities and devices. Diluted Magnetic Semiconductors, specifically, Mn-doped III-V compounds, offer unique features that allow for precise modulation of carrier spin dynamics, a crucial aspect for the advancement of spintronic devices [1]. One prominent application of these materials is in the field of Magnetic Random Access Memory (MRAM), where they enable efficient spin injection and manipulation [2]. Mn-doped III-V compounds have also found applications in magneto resistive sensors, such as Tunnelling Magneto-Resistance (TMR) and Giant Magneto-Resistance (GMR) sensors to detect and amplify magnetic fields [3,4]. They also hold promise for advanced mass storage devices like hard disks, as they allow for precise spin orientations manipulation and detection [5].

Researchers are actively investigating GaMnP's potential for spin injection, spin manipulation and spin detection, which are fundamental components of spintronic systems. This exploration is focused on establishing the connection between DMS materials and spintronics. S.J. Pearton et al., [6] synthesized ferromagnetic GaMnN and GaMnP compounds at high temperatures to prevent amorphization and enhance their magnetic properties. Iftibhar Ahmed et al., [7] used the FP-LAPW method to investigate the spin polarization of GaMnP and GaMnAs at x = 0.125. Y. Yuang et al., [8] examined the structural transport and magnetic properties of GaMnP with varying Mn concentrations using pulsed laser annealing (PLA) and ion implantation. A. Laref et al., [9] conducted calculations on hexagonal $GaN_{1-x}P_x$, revealing direct energy gaps and strong polarization dependence in their optical properties, making them promising for solar-cell applications. Z. Young-Zhi et al., [10] found room temperature ferromagnetism in GaAs and GaP compounds doped with V, Cr and Mn atoms at a concentration 25%. J. Mašek et al., [11] focused an investigation the electronic structure of Mn doped Ga(P,As) and (Ga,Al)As materials in the ferromagnetic state. W. Sukkabot., [12] studied magnetism in GaP with transition metal doping using spin density functional calculations. Co and Fe dopants transformed GaP into metal while V retained semiconducting with a reduced band gap. K. Kirandish et al., [13] explored the effect of the pressure on the properties of $Ga_{0.75}Cr_{0.25}P$ utilizing the SIESTA code (Spanish Initiative for Electronic Simulations with Thousands of Atoms). P. Mahadevan et al., [14] delved into the inherent mechanism of ferromagnetism in GaAs, GaP, GaN and GaSb diluted magnetic alloys with Mn substitution focusing on the analysis of the electronic structure trends. N Benbouchi et al., [15] applied spin-dependent density functional theory to study Co doping in GaP,

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revealing that Co-doped GaP for spin-based electronic applications due to their complete half-metallic properties and integer total magnetic moments.

Exchange and correlation interactions exert a substantial effect on the distinct properties and behaviors of semiconductors. The exchange interaction reflects the tendency of electrons to align their spins. Meanwhile, the correlation interaction refers to the influence of electrons on each other, impacting the electronic structure and transport characteristics.

This paper investigates the impact of these interactions on the spin polarization of $Ga_{0.75}Mn_{0.25}P$ electronic structure and magnetic properties in the B3 Zinc Blende phase. The study utilizes the Density Functional Theory (DFT) with onsite exact-exchange functional, incorporation variations in the HF exchange parameter (α) ranging from 0 to 25%.

METHOD OF CALCULATIONS

The calculations were conducted utilizing the WIEN2k computer package, employing the FP-LAPW method (Full Potential Linearized Augmented Plane Wave) [16,17]. For spin polarized calculations, the PBE+E parameterization was used, which combines for the PBE (Perdew, Burke and Ernzerhof [18]) method with an onsite exact-exchange treatment for correlated electrons. This approximation effectively considered the exchange and correlation effect. The onsite exact-exchange energy expression as defined by Novák et al [19] can be represented as:

$$E_{XC}^{DFT+E} = E_{XC}^{DFT+E}[\rho] + (\alpha E_{XC}^{HF}[\varphi] - E_{XC}^{DFT}[\rho]). \quad (1)$$

Where (ρ) represents the electron density, (φ) denotes the wave function and (α) signifies the fraction of HF exchange, which can take on either a short-range or long-range value [20]. The long-range value of HF exchange up to 50% is required to obtain acceptable thermo chemistry for the Local Spin Density Approximation (LSDA) [21]. In the Generalized Gradient Approximation (GGA) of PBE, typically uses a short-range value of α=0.25 it has been theoretically deduced and this choice has proven notable success [22,23].

The wave functions and potential are expanded using Muffin-tin approach with a cutoff $I_{max} = 9$. For the Interstitial Region (IR), a cutoff $R_{min} = 8$ is employed. The chosen cut-off energy is 10^{-3} Ryd which separates core states from valence states. For first-consistent results, 1000 k-points are used in the first Brillouin zone.

The crystal structure of $Ga_{0.75}Mn_{0.25}P$ was generated using eight atoms super cell with dimensions 1×1×1. Specifically, the Mn atom replaced the Ga atom located at the position (0,0,0). The atomic spheres radii for Ga, Mn and P were set to 1.95, 1.99 and 1.55 respectively. The total energy was optimized by adjusting the volume of the super cell utilizing the Package of Two-Dimensional Optimize [24].

RESULTS AND DISCUSSION

Structural properties

To determine the ground state of the $Ga_{0.75}Mn_{0.25}P$ compound, The Murnaghan's equation of state [25] is employed for the purpose of fitting to calculate the total energy in term of its volume. This calculation is performed for ferromagnetic state using PBE+E approximation.

The resulting values for various structural parameters of $Ga_{0.75}Mn_{0.25}P$ such like the Lattice Parameter (LP), the Volume (V), the Bulk modulus (B), derivative of bulk modulus (B') and the Total Energy (E_{Tot}) show observable convergence with other data [26-28] presented in Table 1.

Table 1. Structural properties of $Ga_{0.75}Mn_{0.25}P$ at different values of HF exchange parameter (α)

α	LP (Ang)	V (Ang^3)	B (GPa)	B'	E_{Tot} (Ryd)
0	5.493 5.49[26]	165.719	79.03 88.61[26]	4.894 4.68[27]	-16718,973 -16718.97441[28]
0.05	5.571	172.882	76.86	4.487	-16718,97859
0.10	5.629	178.364	53.64	5.257	-16718,98954
0.15	5.690	184.301	67.58	5.201	-16719,00784
0.20	5.787	193.854	70.18	4.733	-16719,05385
0.25	5.854	200.687	82.46	5.051	-16719,0992

Figure 1 demonstrates that as exchange and correlation interactions increase, both the LP and Volume of $Ga_{0.75}Mn_{0.25}P$ increase. This indicates significant influence of these interactions on the unit cell size. Specifically, exchange and correlation interactions directly affect the equilibrium positions of atoms and their bonding behavior within the unit cell, ultimately leading to an expansion of the unit cell size.

Figure 2 shows that increasing exchange and correlation interactions lead to a significant decrease in total energy of $Ga_{0.75}Mn_{0.25}P$. These interactions strongly influence the electronic properties by modifying the distribution and behavior of electrons, resulting in a pronounced reduction in total energy.

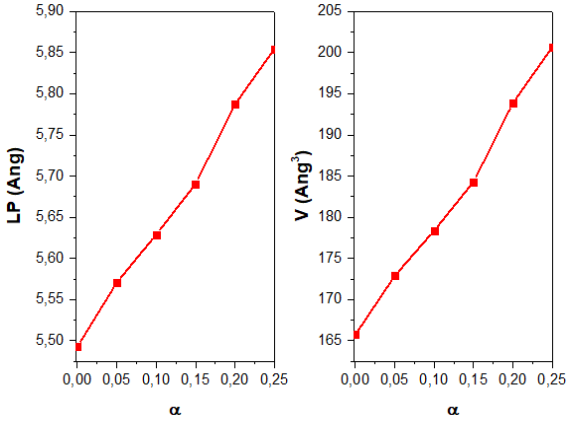

Figure 1. Influence of exchange and correlation interactions on lattice parameter (LP) and volume (V) of $Ga_{0.75}Mn_{0.25}P$

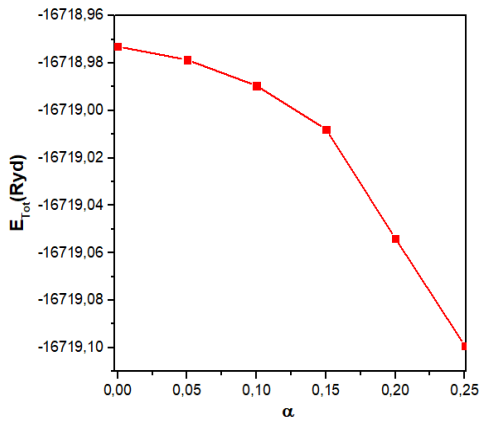

Figure 2. Influence of exchange and correlation interactions on total energy (E_{Tot}) of $Ga_{0.75}Mn_{0.25}P$

Electronic properties

The spin polarized band structures of $Ga_{0.75}Mn_{0.25}P$ have been computed within the first Brillouin zone. Figure 3 depicts that the electrons in the spin up (↑) state outnumber those in the spin down (↓) state. There is a band gap present around the Fermi level (Ef) for spin down state, while a few valence bands in the spin up state intersect the Fermi level and transition into the conduction band. Consequently, based on the occurred interactions range of 0 to 25%, $Ga_{0.75}Mn_{0.25}P$ compound is predicted to exhibit metallic behavior for spin up state and semiconductor behavior for the spin down state. Further investigation indicates that this compound is a half metallic ferromagnetic material.

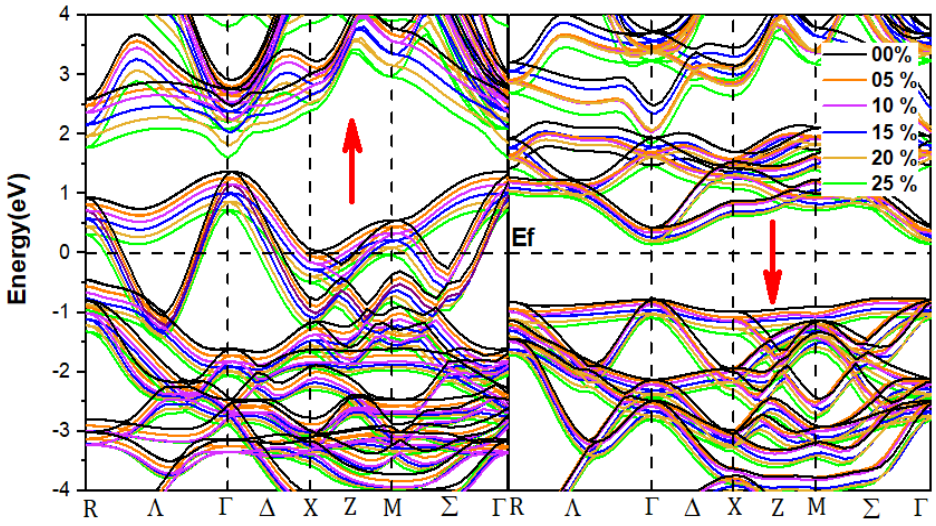

Figure 3. Influence of exchange and correlation interactions on spin polarized band structures of $Ga_{0.75}Mn_{0.25}P$

In the Figure 4, the calculated band structures highlight a noticeable increase in the forbidden energy gap (Eg) for spin down state. This increase is attributed to significant changes in the maximum of the conduction band and the minimum of the valence band, resulting from the increasing exchange and correlation interactions.

The calculated electronic properties are summarized in Table 2, it includes conduction band minimum of spin down state and spin up state ($E_{CBM}^{up}, E_{dn}^{CBM}$), valence band maximum of spin down state and spin up state ($E_{VBM}^{up}, E_{dn}^{VBM}$), the band edge spin splitting (ΔEc) for the conduction band minimum and the band edge spin splitting (ΔEv) for the valence band maximum are determined using specific formulas:

$$\Delta Ec = E_{CBM}^{up} - E_{dn}^{CBM}, \tag{2}$$

$$\Delta Ev = E_{VBM}^{up} - E_{dn}^{VBM}. \tag{3}$$

These formulas are commonly used to analyze band structure and determine various properties of electronic states at (Γ) symmetry point.

In the Figure 4, the calculated band structures highlight a noticeable increase in the forbidden energy gap (Eg) for spin down state. This increase is attributed to significant changes in the maximum of the conduction band and the minimum of the valence band, resulting from the increasing exchange and correlation interactions.

Table 2. Electronic properties of $Ga_{0.75}Mn_{0.25}P$ at different values of HF exchange parameter (α)

α	0	0.05	0.10	0.15	0.20	0.25
Eg_{dn} (eV)	1.20013 1.20[28]	1,20218	1,20973	1.21289	1,22001	1,22857
E_{VBM}^{up} (eV)	0	0	0	0	0	0
E_{dn}^{VBM} (eV)	-0,77277	-0,80629	-0.86033	-0,95136	-1,02482	-1.08531
E_{CBM}^{up} (eV)	0	0	0	0	0	0
E_{dn}^{CBM} (eV)	0,42736	0,39589	0.3494	0,26153	0,19519	0.14326
ΔEv (eV)	0,77277	0,80629	0.86033	0,95136	1,02482	1.08531
ΔEc (eV)	-0,42736	-0,39589	-0.3494	-0,26153	-0,19519	-0.14326

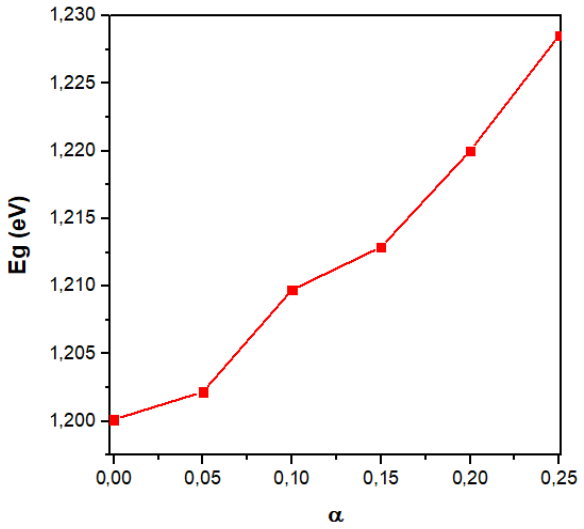

Figure 4. Influence of exchange and correlation interactions on band gap energy (Eg) of $Ga_{0.75}Mn_{0.25}P$

Magnetic properties

Upon substituting Ga atoms with Mn in GaP, the resulting GaMnP compound exhibits magnetic properties attributed to Mn-3d. The coupling between the 3d orbital of Mn and the 3p orbital of P atoms results in the emergence of small local magnetic moments in both Ga and P atoms. Notably, for $Ga_{0.75}Mn_{0.25}P$, the local magnetic moment of P exhibits a negative value, indicating an anti-parallel alignment with the Mn spin, whereas the positive value observed on Ga signifies a parallel alignment.

Figure 5 illustrates the variation of the both local and total magnetic moments of $Ga_{0.75}Mn_{0.25}P$ under the influence of exchange and correlation interactions. As the interactions increase, the total magnetic moment remains constant at 4.00 μB. Nonetheless, the magnetic moment of Mn atom increases, whereas the local magnetic moments at P and Ga atoms decrease. These findings are in agreement with other data [29] presented in Table 3.

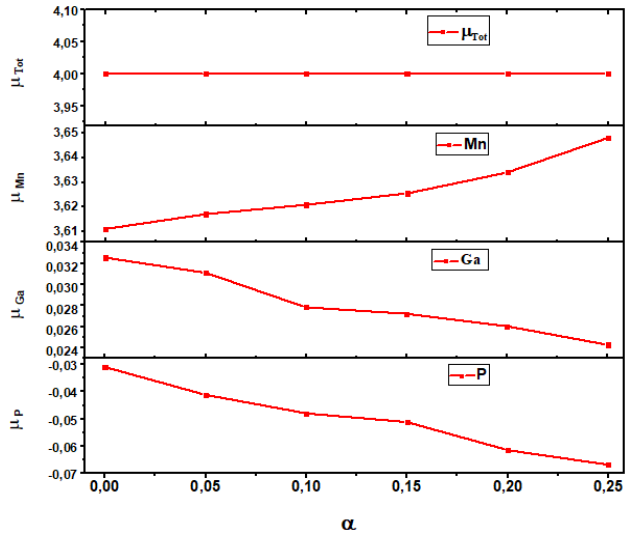

Figure 5. Influence of exchange and correlation interactions on magnetic moment μ_{Tot}, μ_{Mn}, μ_{Ga} and μ_P of $Ga_{0.75}Mn_{0.25}P$.

Table 3. Magnetic properties of $Ga_{0.75}Mn_{0.25}P$ at different values of HF exchange parameter (α)

α	μ_{Mn} (μB)	μ_{Ga} (μB)	μ_{P} (μB)	μ_{Tot} (μB)
0	3,61121 3,382[29]	0,03255 0,023[29]	-0,03091 -0,039[29]	4,00042 4,05[29]
0.05	3,61718	0,03112	-0,04114	4,00068
0.10	3,62101	0,02784	-0,0479	4,00068
0.15	3,62559	0,02723	-0,05113	4,00068
0.20	3,63412	0,02603	-0,06142	4,00068
0.25	3,64813	0,02428	-0,06673	4,00068

CONCLUSIONS

The interactions studied affect the structural properties of $Ga_{0.75}Mn_{0.25}P$ by increasing the lattice parameter and volume, and decreasing the total energy. The electronic structures show a downward shift of the valence and conduction bands, resulting in an increased band gap. The compounds exhibit half metallic ferromagnetism within the range of 0 to 25% of HF exchange. The magnetic properties indicate a noteworthy phenomenon in which the coupling between the 3d orbital of Mn and the 3p orbital of P atoms induces local magnetic moments in the Ga and P atoms. Moreover, as the interactions strength intensifies, the magnetic moment of Mn atom increases, while it decreases on Ga and P atoms. However, it is important to note that despite these changes, the total magnetic moment remains unchanged.

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ВПЛИВ ОБМІННОЇ ТА КОРЕЛЯЦІЙНОЇ ВЗАЄМОДІЙ НА СПІНОВУ ПОЛЯРИЗОВАНУ ЕЛЕКТРОННУ СТРУКТУРУ ТА МАГНІТНІ ВЛАСТИВОСТІ $Ga_{0,75}Mn_{0,25}P$ У СТРУКТУРІ ЦИНКОВОЇ ОБМАНКИ B3

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Це дослідження зосереджено на вивченні впливу обмінних і кореляційних взаємодій на спін-поляризовану електронну структуру та магнітні властивості $Ga_{0.75}Mn_{0.25}P$ у фазі B3 Zinc Blende. Розрахунки першого принципу були виконані шляхом систематичної зміни значення обміну Хартрі-Фока (HF) (α) від 0 до 25% з використанням локального функціоналу точного обміну для обрахунку поведінки корельованих електронів. Електронні та магнітні властивості показують, що $Ga_{0.75}Mn_{0.25}P$ демонструє напівметалеву феромагнітну поведінку при різних значеннях HF-обміну. Крім того, зі збільшенням параметра фракції (α) ширина забороненої зони збільшується, що призводить до модифікацій у спін-поляризованих зонах структурах. Крім того, наші дослідження показують, що обмінні та кореляційні взаємодії викликають збільшення параметра решітки та об'єму сполуки. Крім того, ці взаємодії призводять до зменшення магнітних моментів атомів P і Ga, тоді як моменти Mn збільшуються. Ці висновки дають цінну інформацію про поведінку $Ga_{0.75}Mn_{0.25}P$ для потенційних застосуваннь в дизайні спінтронних пристроїв.

Ключові слова: *ВЧ-обмін; корельовані електрони; GaMnP; магнітний матеріал; напівметалічний; спінтроніка*