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Posted Date: 9 January 2025

doi: 10.20944/preprints202501.0667.v1

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Article

Electronic Correlations in Ferromagnetic Heusler Alloy In_2MnW : Insights from First-Principles Calculations

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Abstract: First-principles calculations are performed to examine the physical features of full Heusler In_2MnW . The WIEN2K code is utilized with the variety of approximations, including the GGA and GGA + U, to examine the structural, electronic, and magnetic properties. The unit cell is optimized to achieve the ground state energy level. The calculated ΔH for In_2MnW is -0.189 eV. This negative ΔH value signifies the thermodynamic stability of the compound. The metallic behavior of the investigated compound is confirmed by the calculated band structure (BS) with both potentials. These potentials are also used to calculate the total density of the state, which confirm their metallic nature. Total magnetic moment value is recorded as 4.3 μ_B while addition of U parameter slightly enhances its value to 4.4 μ_B . These studied properties indicate that In_2MnW has a metallic ferromagnetic character and is ideally appropriate for the usage of mass storage devices as a ferromagnetic material

Keywords: Heusler alloys; ferromagnetic materials; first principles calculations; electronic properties; structural stability

1. Introduction

The Heusler alloys, first discovered in 1903 [1], have demonstrated remarkable properties that have led to widespread commercial applications in various devices, including energy harvesters [2] and magnetic read access memories (MRAM) [3], sensors, spintronics, actuators [4,5], thermoelectric materials [6–8], solar cells [9,10], and semiconductor materials [11]. Heusler materials are also promising for gadgets such as hard disks, optical discs, and magnetic disk drives [12]. Heusler alloys typically consist of two parts manganese, one section copper, and other tin. These materials belong to the family of Heusler alloys, characterized by the empirical formula X_2YZ , comprising three intersecting FCC sublattices (in space group $Fm\bar{3}m$) [13]. Symmetry breaking (in the non-centrosymmetric space group $F\bar{4}3m$) divides the X_2 lattice, originally with a multiplicity of 8, into two sublattices with a multiplicity of 4 each, wherein one sublattice remains unoccupied, leading to the formula XYZ in half-Heusler phases [14].

The pursuit of novel materials is witnessing an exponential surge as scientists strive to advance technology for the betterment of humanity. Among these materials, Heusler alloys stand out, captivating researchers' attention. Dahal and Kaphle [15] studied the physical features of XYZ -type half-Heusler materials. They found that most spin channels exhibit certain band gaps (E_g), such as 0.38 eV for FeMnGe and 0.95 eV for CoMnSb , indicating that present Heusler alloys possess half-metallic nature. Fiedler and Kratzer [16] conducted first-principles calculations utilizing the PBE and HSE06 exchange functionals on ternary NiZrSn and CoZrBi semiconductors with the C_{1b} crystal structure. Their study involved calculating the fundamental structural, electronic, and phonon properties using density functional theory. Wakeel et al. investigated the physical features of Pd_2AZ

(A = Cu, Hf, Mn, Ti, Zr; Z = Al, Ga, In, Sn) by utilizing the DFT computations. All these Heusler materials were found to be metallic due to the overlapping of valence and conduction bands [17].

As our study progressed, we uncovered a wealth of insights into the physical properties of Heusler In_2MnW . From its magnetic behavior to its electronic structure, each revelation added a new layer to our understanding. With each discovery, the allure of this compound grew, beckoning us to delve deeper into its complexities. Our findings not only shed light on the fundamental properties of Heusler In_2MnW but also opened doors to a multitude of potential applications. With this newfound knowledge, we stand on the brink of a new era in Heusler In_2MnW research, poised to unlock its full potential and explore the boundless possibilities it holds.

The entire metallic cubic structure of the Heusler In_2MnW combination served as the basis for our investigation. According to our estimates, magnetic moment is essential to making the In_2MnW combination workable for magnetic materials. Up until our literature review of the material, the theoretical In_2MnW compound had never been studied. This paper's remaining material is broken up into multiple sections. Section 2 defines the computational examination of a chemical. The structural, lattice parameters, electrical, and magnetic characteristics of the In_2MnW compound are examined in Sect. 3. Finally, Sect. 4 describes the conclusions.

2. Computational Method

First-principles computations were performed to investigate the physical features of the full Heusler In_2MnW using the WIEN2K code [18] within DFT. The full potential linearized augmented plane wave (FP-LAPW) [19] method was employed in these calculations. The Kohn-Sham equation was solved to determine the ground state characteristics, focusing on the minority electrons necessary for calculating these parameters. The Generalized Gradient Approximation (GGA) [20] and GGA+U potentials were used in the study. The GGA+U potential, incorporating an intramolecular Coulombic repulsion term, was found to be the best method for accurately unfolding the localized d and f electrons. For the In_2MnW , an effective U (U_{eff}) value of 7 eV was used to handle the d and f states. This approach accounts for the self-interaction error in the d states of the orbitals, particularly for the partially filled d states in In and Mn (transition elements). The calculation method involves dividing the entire crystal into distinct muffin-tin (MT) spheres divided by an interstitial region. Within the MT spheres, a basis set is expanded using spherical harmonic functions, while plane waves are used in the interstitial region. The R_{MT} were calculated to be 2.5 atomic units (au) for Mn, W, and In. A core-valence separation energy of -11 Rydberg (Ry) was used to prevent charge diffusion from the MT spheres [21]. For energy convergence, the wave function cut-off parameter was set to $K_{\text{max}}R_{\text{MT}} = 5$, where R_{MT} is the smallest muffin-tin radius and K_{max} is the plane wave expansion parameter. A mesh of 1000 k-points was also used for the Brillouin zone (BZ) to ensure accurate results. The total energy convergence criterion was set to less than 10^{-6} Ry.

3. Results and Discussion

3.1. Structural Properties

The Heusler compound In_2MnW has a cubic crystal structure with the space group Fm-3m (No. 225) as described by Graf et al. (2009) [22]. In this structure, the In atoms are positioned at coordinates (0.25, 0.25, 0.25) and (0.75, 0.75, 0.75), while Mn and W atoms are positioned at (0, 0, 0) and (0.50, 0.50, 0.50) correspondingly within the unit cell. Figure 1(a) illustrates the atomic positions within the primitive cell. The compound exhibits a three-dimensional Heusler structure and an L2₁-type configuration. In this FM Heusler alloy, W is bonded to four equivalent Mn atoms and ten In atoms in a distorted body-centered cubic arrangement. The bond lengths between W and Mn atoms are 2.86 Å and 2.88 Å, while the W-In bond lengths range from 2.86 Å to 3.33 Å. Mn is bonded to four equivalent W atoms and four equivalents In-atoms, with Mn-In bond lengths ranging from 2.86 Å to 2.87 Å. There are two distinct In sites in the structure. In the first site, In is bonded to four equivalent W atoms and four equivalent In atoms, forming distorted edge-sharing InIn_4W_4 tetrahedra. In the

second site, In is bonded in a 4-coordinate geometry to six equivalent W atoms, four equivalent Mn atoms, and four equivalent In atoms. Optimization of the crystal structure is crucial for determining the stability, band gap structure, and carrier transport properties of the material. The lattice parameters are optimized by minimizing the total energy within the Fm-3m symmetry space group. The energy-volume optimization curve is shown in Figure 1. The primary goal of this optimization is to confirm the stability of the selected compounds and ensure their suitability for the properties being studied. Additionally, optimizing the compounds is essential as density functional theory (DFT) provides accurate results at the ground state, making it necessary to refine the structures under investigation. To determine the structural parameters, we used the Birch-Murnaghan equation. Additionally, we examined the lattice atomic positions and cell dimensions to determine the compound's structural morphology. The Birch-Murnaghan equation is given as [23]:

$$E(V) = E_0 + \frac{9V_0B_0}{16} \left[\left\{ \left(\frac{V_0}{V} \right)^{2/3} - 1 \right\}^2 B' + \left\{ \left(\frac{V_0}{V} \right)^{2/3} - 1 \right\} \left\{ 6 - 4 \left(\frac{V_0}{V} \right)^{2/3} \right\} \right] \quad (1)$$

Our optimization results indicate that the ferromagnetic (FM) phase is the most favorable for In_2MnW compared to the paramagnetic (PM) and antiferromagnetic (AFM) phases. The formation energy (ΔH) is calculated as the difference between the total energy (E_0) of In_2MnW and the sum of the individual energies of In, Mn, and W (E_{In} , E_{Mn} , and E_{W} , respectively). It can be computed as [24]:

$$\Delta H = E_{\text{In}_2\text{MnW}} - 2E_{\text{In}} - E_{\text{Mn}} - E_{\text{W}} \quad (2)$$

where, $E_{\text{In}_2\text{MnW}}$ signifies the total energy of In_2MnW , while E_{In} , E_{Mn} and E_{W} represent the optimized total energy of the respective atom. The value of ΔH was computed as -0.189 eV for In_2MnW . The negative value of the ΔH indicates that it is thermodynamically stable [21].

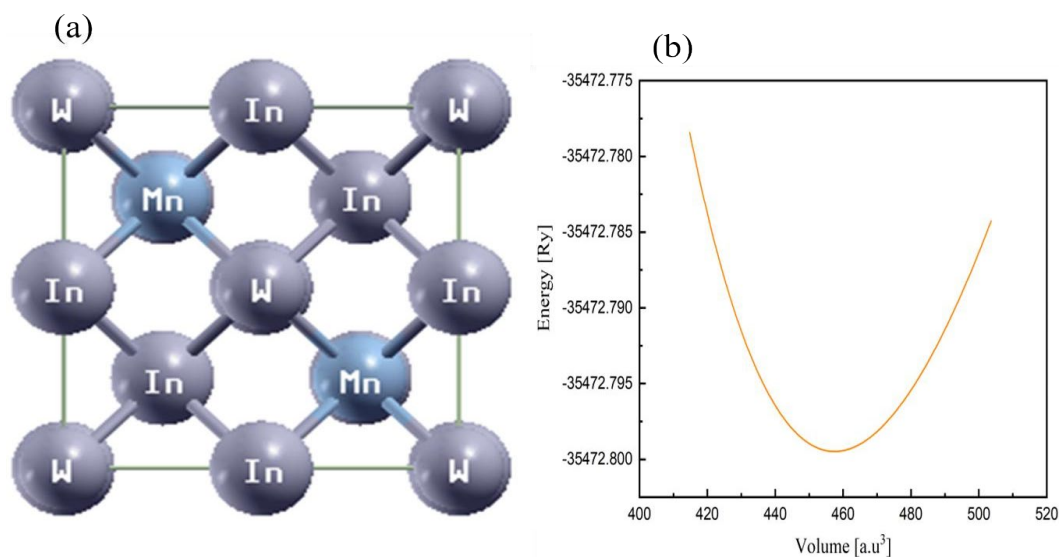


Figure 1. Illustration of (a) compound structure and (b) volume optimization curve of In_2MnW .

3.1.1. Lattice Parameters

We have optimized the structure of In_2MnW to study the ground state properties. The theoretical lattice constants were obtained by minimizing the total energy (E_{TOT}) with respect to the lattice parameter. The purpose of optimization is to make a compound stable in order to make our calculation in ground state energy. The value of lattice parameters for optimized structure are found to be 6.33 Å. We estimated the total energy for dissimilar volumes in the vicinity of the calculated experimental volume to optimize the unit cell and to obtain the ground state energy. Figure 1 (b) shows the optimization curve for total energy against volume. To determine the structural and optimize parameters of material, Birch Murnaghan's is used. This equation shows a relation between volume and pressure of body and gives the material energy as a function of volume. Further the compound structural morphology is determined by examining both the lattice atomic positions and cell dimensions. The ferromagnetic phase (FM) is the most favorable phase for In_2MnW . In addition,

available experimental results, up to our literature review, concluded that the most appropriate phase is ferromagnetic for the material.

The value of formation energy for this compound is negative, which means it is thermodynamically stable. Where total energy of full Heusler In_2MnW , and individual energy of In_2 , Mn and W is E_{In_2} , E_{Mn} and E_{W} respectively. The difference of the total energy E_0 of the compound and individual energy of each element of that compound is known as formation energy. From calculated formation energy, we can predict that our compound is stable. The optimized parameters such as unit cell energy (E_0), bulk modulus B (GPa), lattice constant ($\text{\AA}$) and pressure derivation of bulk modulus (BP) are given in Table 1.

Table 1. Optimized lattice parameters of In_2MnW compound.

Lattice parameters	Lattice constant	V_o	BP	B (Gpa)	E_0		
					PM	FM	AFM
Pd2Mn	6.33	490.1032	5.00	203.9194	-58182.48	-58182.51	-581821.51
Sb	6.413^a						
Exp.^{a,b}	6.420^c						

3.2. Electronic Characteristics

To gain a detailed comprehension of material’s characteristics, the band gap is a crucial factor for visualizing the material’s nature. In this section, we present the comparative analysis of GGA and GGA+U computed electronic properties of In_2MnW Heusler alloy. Previously, no studies have been investigated for both electronic and magnetic properties of In_2MnW . For this purpose, we computed the spin-dependent band dispersions, total (T) and projected (P) density of states for In_2MnW to explore its potential for various electronic devices. Figure 2 and Figure 3 show that the bands profile of the compound under investigation, it can be seen that the band structure of compound lies on asymmetry lines $\Gamma \rightarrow M \rightarrow K \rightarrow \Gamma \rightarrow A$ of the first Brillouin zone. The metallic nature of the compound is evident from these figures. For both spin channels, states overlap the Fermi energy levels, indicating metallic behavior with the respective potentials. This overlap between the VB and CB confirms the compound’s metallic nature. The presence of metallic nature in both spin channels predicts that In_2MnW exhibits full metallic ferromagnetic properties. TDOS results indicate that both majority and minority charge carriers are well-aligned with the band structure results. The metallic character enhances the transport of spin-asymmetric current which leads to high spin polarization ratio in the compound which is widely used in ferromagnetic materials.

Furthermore, the interstitial and individual atoms (Mn and In) contribute to the net μ_B of the In_2MnW compound, while the W site opposes it. This observation is based on the measured μ_B values via both approximations. The frequent emergence of Mn/In-d states explains this behavior. The PDOS shows the impact of projected states of Mn, W, and In, highlighting the dominant contributions from these atoms. The p state of In crosses Fermi level in up spin orientation, ensuing the compound’s metallic character. The higher peaks in the vicinity of Fermi level are primarily influenced by d states of Mn and W. It can be concluded that In-p and Mn-d states are the significant contributors to the compound’s electronic properties.

The spin-polarized electron densities of In_2MnW have been plotted along the (110) plane to determine the type of bonding among their constituent atoms, as shown in Figure 4. The spin-up states reveal a covalent link between Mn and In atoms, whereas the bond between Mn and W is ionic. In the spin-down channel, substantial covalency is observed between Mn and In bonds, while the ionic character of Mn and W bonds decreases from Mn to W, which is expected due to changes in atomic size. As the d-bands transition from nearly filled to partially filled, the electron density of Mn changes from a spherical to a dumbbell shape as it moves from spin-up to spin-down.

Calculating the partial density of states (PDOS) provides a clear understanding of the magnetic characteristics. Its magnetic character is indicated by the asymmetric nature of the up and down spins DOS. As can be seen from partial DOS, the orbitals of Mn, In, and W atoms have made a dominant contribution to the contribution of individuals.

Figure 2. The calculated band structure of In_2MnW with spin up and spin down-states by using PBE-GGA potential.

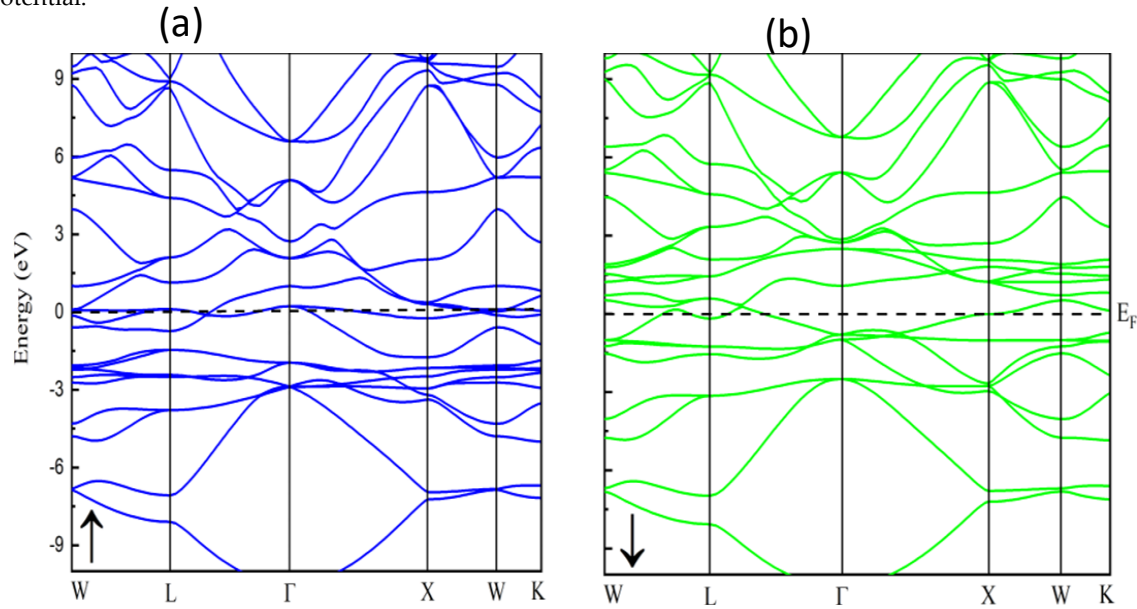


Figure 3. The calculated band structure of In_2MnW with spin up and spin down by using GGA+U potential.

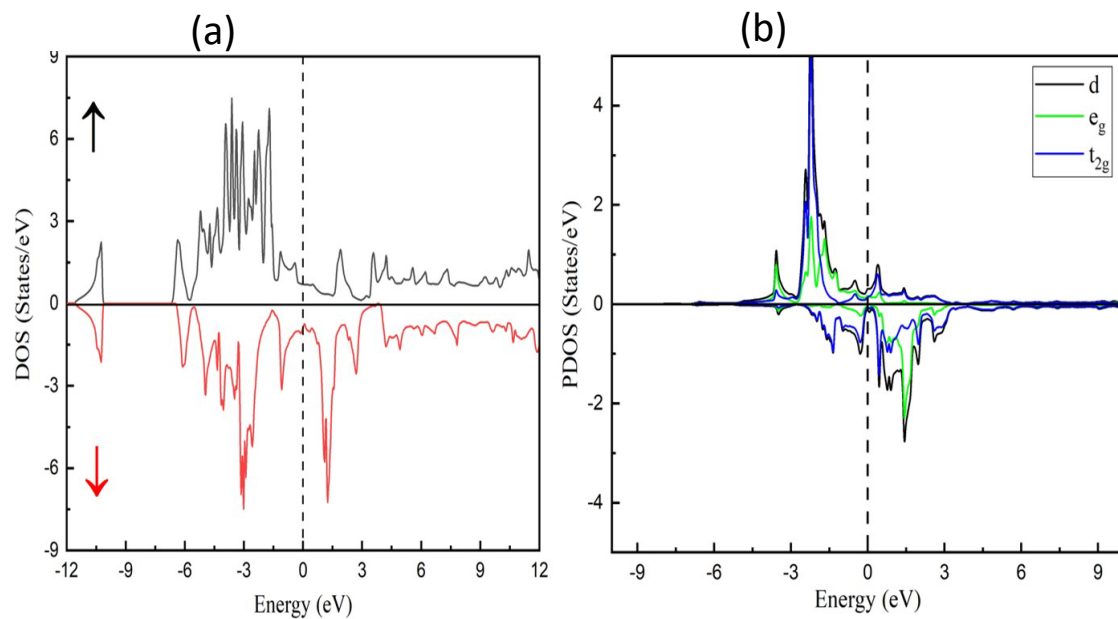


Figure 4. Calculated (a) total and (b) partial densities of states of In_2Mn with GGA spin up and down.

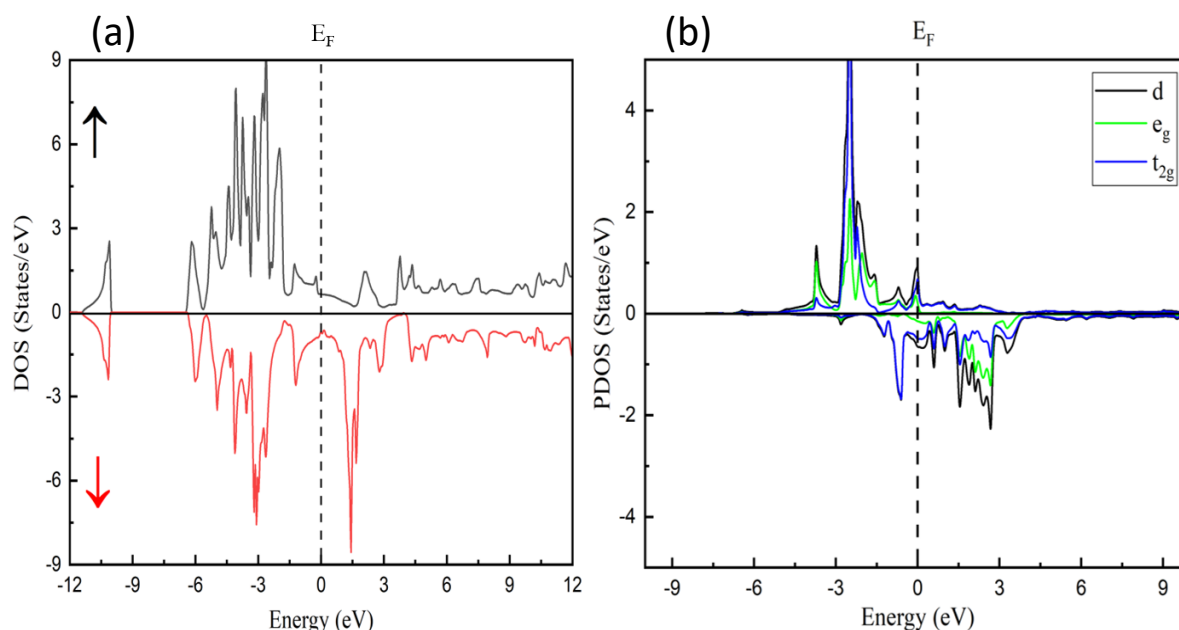


Figure 5. Calculated (a) total and (b) partial densities of states of In_2MnW (illustrating the high exchange splitting) calculated with GGA +U spin up and down.

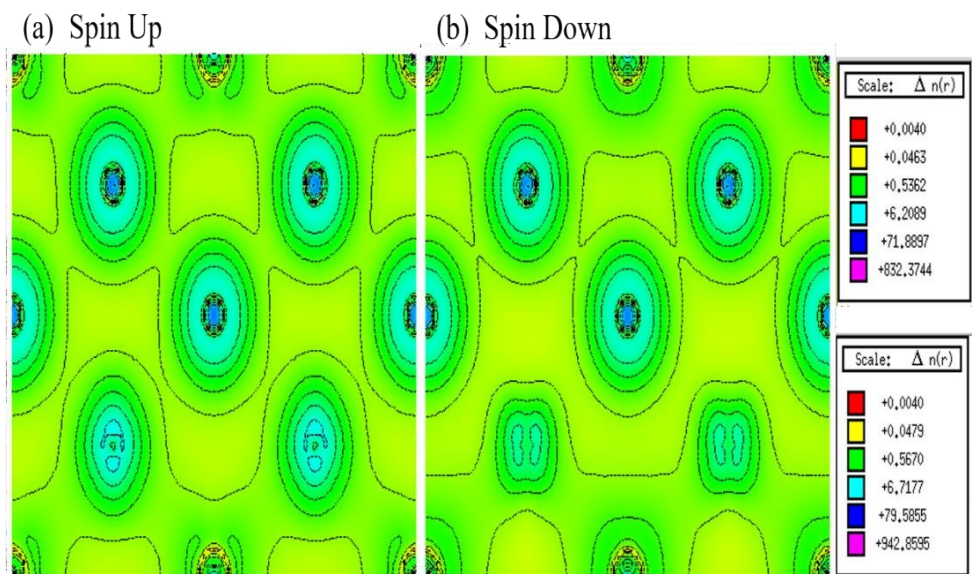


Figure 6. Illustration the Contour plot of In_2MnW .

3.3. Magnetic Properties

The magnetic characteristics of In_2MnW compound have been examined in light of spin based asymmetric electronic states as predicted in electronic properties by discussing TDOS and PDOS plots. The magnetic moments (μ_B) of W, Mn, and In were computed separately using both GGA and GGA+U. The magnetic moment value shows the magnetic characteristics of In_2MnW . The total, interstitial, and individual μ_B of In_2MnW atoms (In, Mn, and W) are summarized in Table 2. The calculated moment values of In_2MnW are ~ 4.30 and ~ 4.40 with respective GGA and GGA+U employed is close in comparison with the experimental measurement. In Heusler compounds, μ_B alignment results from two competing effects: intraatomic energy state's splitting d-orbitals and covalent bonding between atoms. As observed, initial In cation is a close neighbor to the second In atom, leading to a minimal separation distance and a significant direct correlation between d orbitals both metals. In Heusler materials, the introduction of two X cations increases complexity of their

physical attributes. PDOS for In₂MnW indicates that Mn exhibits strong hybridization with W. This incorporation induces band restructuring, mainly driven by the hybridized states consisting of d orbitals of Mn and W transition metals. It is widely recognized that a greater μ_B correlates with a strengthened exchange coupling [25]. Mn atoms exhibit a significantly stronger μ_B compared to In and W atoms. The negative μ_B of In atoms is responsible for their diamagnetic behavior, indicating an anti-parallel alignment that affects the overall ferromagnetic direction [26,27]. Consequently, W atoms influence the ferromagnetic nature of the In₂MnW compound. The opposite signs of the μ_B of the interstitial site, Mn, W, and In atoms compared to the total μ_B of the In₂MnW, suggest that electrons VB interact in an anti-parallel manner with the total μ_B of the compound. The results show that In₂MnW exhibits FM behavior due to its strong magnetic features.

Table 2. Total, interstitial, and localized magnetic moment values for In₂MnW.

Parameter	GGA	GGA +U
Total magnetic moment	4.33	4.408
Magnetic moment of Mn	4.1	4.1
Magnetic moment of W	-0.02600	-0.02500
Magnetic moment of In	0.17218	0.15
Interstitial	0.17218	0.083

4. Conclusions

This study employs DFT calculations using with and without Hubbard potential to investigate the structural, electronic, and magnetic properties of the In₂MnW. We confirm that the In₂MnW compound has a cubic geometry exhibiting Fm3m space group. Further, we calculated the electronic properties with GGA and GGA+ U that revealed the metallic behavior of In₂MnW. We calculated the partial density of states to investigate the particular contribution of different states. A key property of interest is the compound’s ability to achieve pronounced magnetization under the influence of an applied magnetic force, owing to its metallic characteristics and strong μ_B . The μ_B of In₂MnW is calculated to be 4.33 μ_B with GGA and 4.408 μ_B with GGA + U, demonstrating its ferromagnetic characteristics in nature. These characteristics make In₂MnW highly suitable for advanced magnetic storage devices.

Data Availability: Data will be made available on request.

Conflict of Interest: Authors declare that there is not any conflict of interest

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