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A first principles study of Palladium-based full Heusler ferromagnetic Pd_2MnSb compound

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Abstract
Density functional theory (DFT)-based calculations were used to calculate the physical properties of the full Heusler compound Pd_2MnSb. The WIEN2K code is used with various approximations, such as generalized Gradient approximation (GGA) and (GGA+U) potentials, to investigate the structural, electronic, and magnetic responses. The unit volume cell is optimized to achieve the ground state energy level. The calculated band structure with both potentials confirms the metallic behavior of the selected compound, Pd_2MnSb. The total density of states is also calculated by using these potentials, which confirms their metallic behavior. The calculated partial density of state with GGA and GGA+U potentials confirmed the particular contribution of atoms. We have calculated the magnetic properties with the GGA and GGA+U potentials to find out the total magnetic moment values that are suitable with the available experimental data. The calculated magnetic moments show that Pd_2MnSb is a magnetized material. These investigated properties show that Pd_2MnSb has metallic magnetized characteristics and is perfectly suitable for the applications of mass storage devices as a ferromagnetic material.

Keywords Density functional theory · Electronic properties · Magnetic Properties · Density of state · Mass storage devices

1 Introduction

In recent years, Extensive theoretical calculations have been done on Heusler compounds because Heusler alloys (Kervan and Kervan 2012) show ability in different applications like Spintronics, Solar cell applications, mass storage devices, and ferromagnetic materials (Berri et al. 2014). Full metallic Heusler compounds are suitable for ferromagnetic materials due to their strong magnetic moment values (Lei et al. 2011). These metallic Heusler compounds are also reliable for mass storage applications like hard drives, magnetic tape, optical disc drives, and magneto-optical disc drives. Full metallic materials are those that exhibit metallic properties in the spin-up channel (Birsan 2014), known as the majority spin carrier, and those that show metallic behavior in the spin-down channel, known as the

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minority spin carrier, which means there is a case of overlapping between the valence band and the conduction band at the Fermi level.

Fritz Heusler (Manna et al. 2018), a German mining engineer and chemist in the nineteenth century, was the inspiration for these alloys. Heusler alloys comprise about two parts manganese, one part copper, and one part tin. Heusler compounds have stimulating magnetic properties. The intermetallic Heusler alloys are defined by two alterations, such as half Heusler having the formula XYZ and full Heusler alloy having the formula X_2YZ. X and Y are normally transition metals, while Z is the foremost class element (Gilleßen and Dronskowski 2009). It has long been realized that the magnetic order observed in Heusler alloys is to a large extent determined by the chemical order and the conduction electron concentration (Webster and Ramadan 1977). Changes in lattice parameters have less significance, in the ordered Heusler structure the Mn atoms are located on an f.c.c, and sub-lattice with a lattice parameter ~ 6 Å and nearest Mn-Mn distances ~ 4.2 Å (Webster and Ramadan 1977). This is normally considered to be too large for direct exchange, and so several indirect s-d exchange mechanisms of RKKY, modified RKKY type, and also super exchange have been postulated as possible exchange mechanisms. Some degree of success has been achieved in fitting the various models to the experimental data (Webster and Ramadan 1977).

Ternary intermetallic compounds containing Mn and Sb and another transition metal T, such as Cu, Ni or Pd, form the $C1_b$ structure at the composition TMnSb and the $L2_1$ (Heusler) structure at the composition T_2MnSb (Webster and Ziebeck 1980) have been experimentally investigated. The compounds are magnetically ordered with moments of about 4 located at the Mn sites (Webster and Ziebeck 1980). Further the pressure effect on the Curie temperature of the ferromagnetic Heusler alloys Au_2MnAI, Pd_2MnSn and Pd_2MnSb are studied under hydrostatic pressure up to 9 kbar and the results are also discussed by taking account of the degree of the atomic order. The Curie temperatures of these Heusler alloys were found to increase linearly with applied pressure in the pressure range investigated. The values of $(1/T_c)$ (dT_c/dP) and T_c determined in the experimental measurements (Shirakawa et al. 1987).

Our purpose of investigation is to deeply study the band gap structure, density of states, and partial density of states, as well as the magnetic moment values of Pd_2MnSb. By nature, the instruction of ferromagnetic (FM) Heusler alloys is always typical and steep in feeble practical magnetic fields. When the magnetic moment is accepted in Mn atoms, as it frequently is in the Heusler alloys X_2MnZ, a value near to is typically detected. Though these are metals, compounds have the ideal model, and localized magnetic properties (Dahmane et al. 2016) are systems for learning the effects of changes in the electron attentiveness on magnetic properties in atomic disorder. In order to expose the character of spin of (Z) and 3d (X) atoms arranged in the magnetic properties of Heusler alloy compounds, wide magnetic and extra capacities have been achieved on quaternary Heusler alloy compounds. It is observed that the spin of electron attentiveness is primarily.

Kulkova et al. (2006) calculated first principles calculations, the electronic structure of full and half Heusler alloy compounds employing FLAPW method. It was discovered that the obtained equilibrium lattice limits and magnetic moments are well determined by available experimental data. Apart from metallic Heusler compounds, half metallic Heusler compounds have a lot of interaction due to their feasibility in many applications like spintronics (Munir et al. 2021). In case of a half metallic Heusler compound, the majority spin carrier

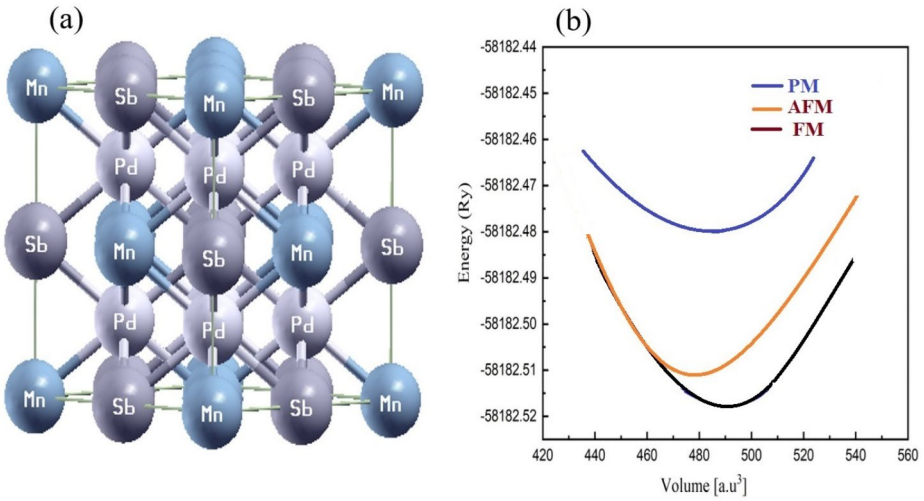

Fig. 1 Illustration of **(a)** compound structure and **(b)** volume optimization curve

Table 1 Optimized lattice parameters of Pd_2MnSb compound

Lattice parameters	**Lattice constant a(Å)**	V_o	BP	B(GPa)	E_o		
					PM	FM	AFM
Pd_2MnSb	6.33	490.1032	5.00	203.9194	-58182.48	**-58182.517**	-58182.51
Exp.[a, c]	6.413[a], 6.420[c]	--------	------	--------	---------	----------	----------

[a]Ref. (Webster and Ramadan 1977), [c]Ref. (Shirakawa et al. 1987)

shows metallic behavior, while minority spin carrier shows non-metallic behavior at the Fermi level which means the presence of band gap between valence and conduction bands.

Our study was based on the full metallic cubic structure Heusler Pd_2MnSb compound. In our calculation, magnetic moment plays a vital role in the making Pd_2MnSb compound become practically feasible for the magnetic materials. Theoretically Pd_2MnSb compound has never been investigated up to our literature survey about the material. The remaining portion of this paper is divided into several different sections. In Sect. 2, the computational study of compound is defined. In Sect. 3, structural, electronic, and magnetic properties of Pd_2MnSb compound are investigated. At the end, conclusions are described in Sect. 4.

2 Computational method

Density functional theory (DFT) (Tawfik et al. 2019) calculations were carried out to investigate the physical properties of full Heusler Pd_2MnSb implemented via WIEN2K code (Blaha et al. 2001), These calculations were based on the Full Potential Linearized Augmented Plan Wave (FPLAPW). To obtain ground state properties Kohn-Sham equation (Bauernschmitt and Ahlrichs 1996) is solved. Less interaction of electrons like in ground

state level is necessary for the calculations. For exchange and correlation interaction, we used generalized gradient approximation (GGA) (Zhang and Yang 1998) and (GGA+U) (Liechtenstein et al. 1995; Bengone et al. 2000) potentials to compute the electronics band structure, density of state, partial density of state and magnetic properties. The improved findings are subsequently compared with the mentioned approximations for the best possibilities, particularly for electronic and magnetic properties. The only method to further improve the clarity of presentation of d/f localized electrons is to use the spin polarized (GGA+U) technique, which also includes an on-site Coulomb repulsion. We have used U_{eff} = 7 eV (Murtaza et al. 2021; Zada et al. 2022a, b, c, 2023a, b; Khan et al. 2022a, b, c, d, 2023) for the Pd_2MnSb compound in order to treat only the d and f states. For atoms with a partially filled d or f state, the value of U is set; Pd and Mn (Transition elements) have a partially filled d state on which the GGA+U technique is implemented to account for self-interaction inaccuracy in d states. So, for this purpose, the use of U_{eff} = 7 eV is to bound the d electrons of Mn and Pd atoms for an accurate result. This strategy depends on the fact that the entire crystal is partitioned into non-overlapping muffin-tin (Mu-T) spheres separated by an interstitial region. At this point, a simple basis set function is picked and expanded in support of spherical harmonic functions within MT spheres, and simple plane waves are utilized in the interstitial region as well. The evaluated value of non-overlapping muffin-tin radii is 2.5, 2.5, 2.5 au for (Mn, Sb and Pd) elements correspondingly. To prevent charge leakage out of the muffin tin spheres, the separation energy between core and valence states for the compound Pd_2MnSb is -11 Ry. In order to attain the energy convergence, the wave function in the interstitial region that enlarged with cut off parameters $K_{max}R_{MT}$ = 5. Where RMT is the smallest muffin tin radius and the maximum reciprocal lattice K_{max} is implemented in the plan wave expansion. A 1000 K points were used for the Brillouin zone (BZ) meshing. The total energy convergence norm was set less than 10^{-6} Rydberg.

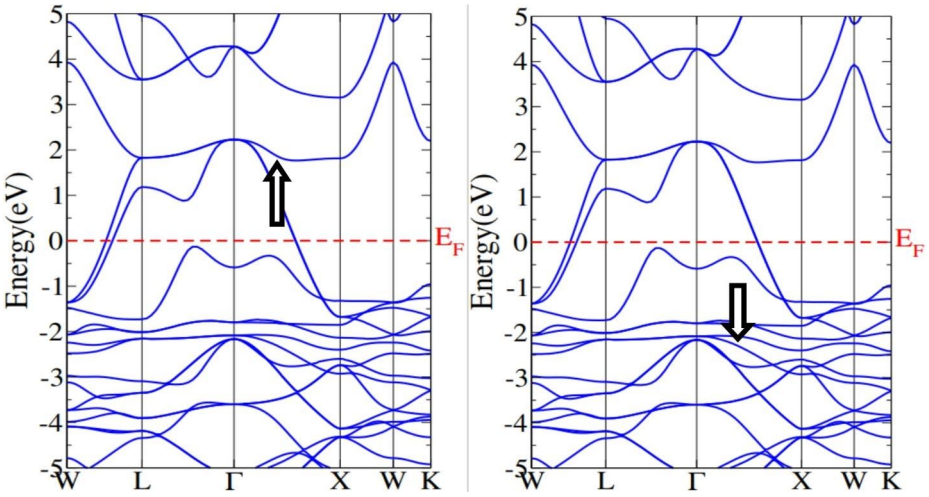

Fig. 2 The calculated band structure with spin up and spin down-states by using PBE-GGA potential

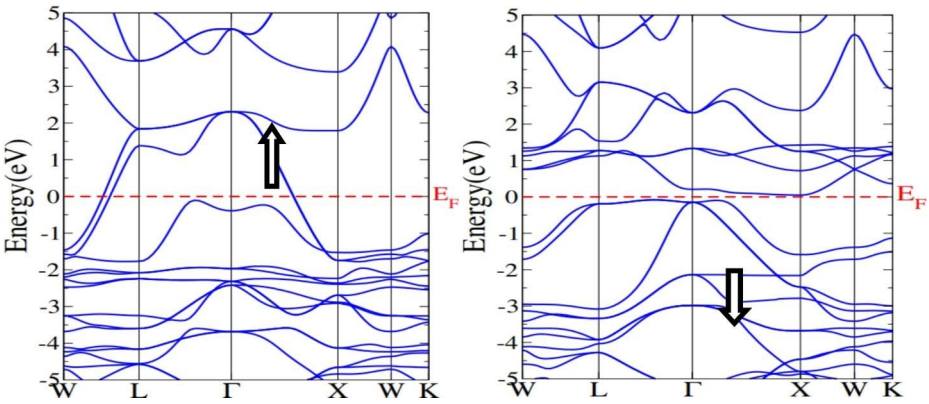

Fig. 3 The calculated band structure with spin up and spin down by using GGA+U potential

3 Results and discussion

3.1 Structural properties

The Heusler compound Pd_2MnSb has a crystal structure (Graf et al. 2009) with the space group Fm-3 m (No. 225). The Pd (0.25, 0.25, 0.25) and Pd (0.75, 0.75, 0.75) are the dissimilar atoms, Mn (0, 0, 0) and Sb (0.50, 0.50, 0.50) occupy the following places in the unit cell. Figure 1(a) depicts the atomic locations occupied by various atoms within the primordial cell. Pd_2MnSb crystallizes in the cubic Fm-3 m space group as mentioned above with three-dimensional Heusler structure. The Ferromagnetic Heusler alloy Pd_2MnSb has the crystal structure with the $L2_1$-type. The Pd atoms occupy the corner site of the bcc structure, while the Mn and Sb atoms occupy alternate body center site (Webster and Ramadan 1977). Webster has once reported that the atomic structure in the alloy Pd_2MnSb has perfect order structure by analysis of neutron diffraction results (Webster 1969). However, the preliminary X-ray studies showed that there is about 10% disorder of Pd and Mn atoms. The results show that there are Mn-Mn pairs with shorter atomic distance which are considered to have negative exchange interaction (Webster and Ramadan 1977; Shirakawa et al. 1987; Webster 1969). The observed small value of the positive pressure derivative of the Curie temperature (dT_c/dP) of the alloy Pd_2MnSb is ascribed to the existence of such Mn-Mn pairs with negative interaction. Optimization of crystal (Krez et al. 2014) is one of the most important factors to find the stability of structure (Larson et al. 2000) and also play an effective role to determine the structure stability, band gap structure and material carrier transport performance for a suitable application.

3.1.1 Lattice parameters

We have optimized the structure of Pd_2MnSb 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

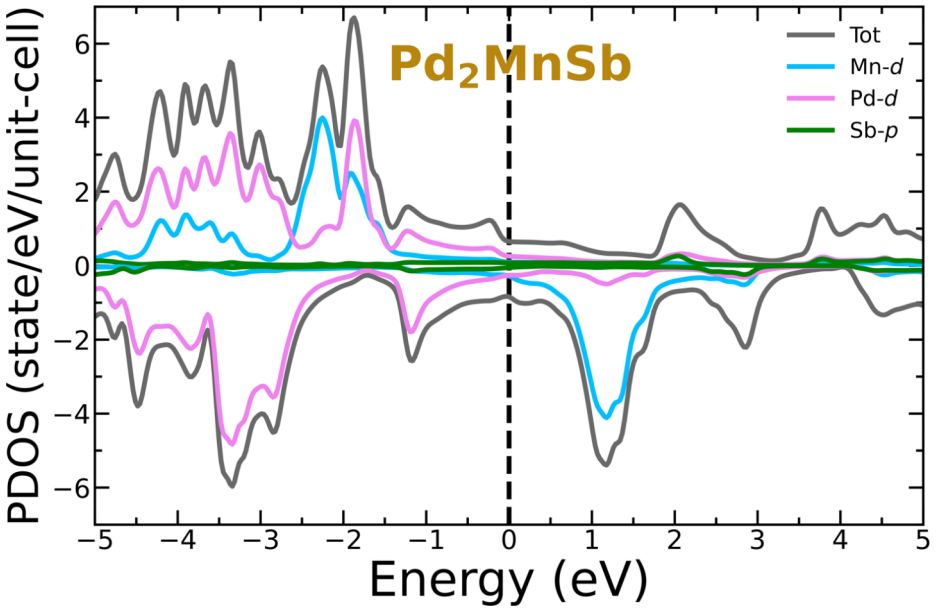

Fig. 4 Shows total and partial density of states with GGA respectively

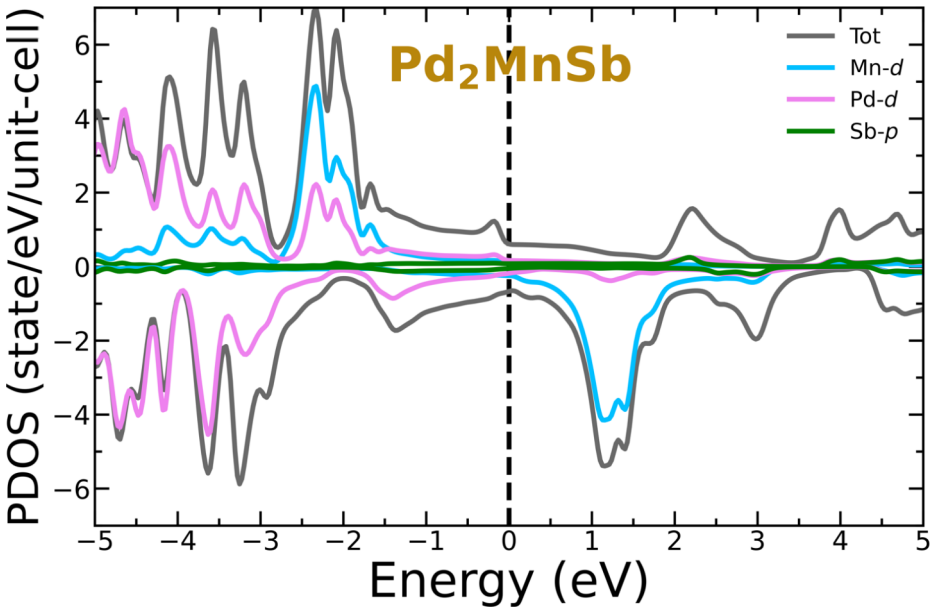

Fig. 5 Shows total and partial density of states with GGA+U respectively

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 Pd_2MnSb as compared to PM and AFM, based on optimization result. In addition, available experimental results, up to our literature review (Webster and Ramadan 1977; Shirakawa et al. 1987), 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 (Kervan and Kervan 2013). Where total energy of full Heusler Pd_2MnSb, and individual energy of Pd_2, Mn and Sb is E_{Pd2}, E_{Mn} and E_{Sb} respectively. The difference of the total energy E_o 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_o), bulk modulus B(GPa), lattice constant (Å) and pressure derivation of bulk modulus (BP) are given in Table 1.

3.2 Electronic properties

To understand the material characteristics, band gap (Li et al. 2009) is essential feature to recognize the material nature. The electronic and magnetic properties of Pd_2MnSb type structure were calculated, previously no studies have been explored for both electronic and overall magnetic properties of Pd_2MnSb. We calculated the spin polarized electronic band structure, total density of state (TDOS) and partial density of state (PDOS) for Pd_2MnSb. In Figs. 2 and 3 it can be seen that the band structure of compound lies on asymmetry lines Γ→M→K→Γ→A of the first Brillouin zone. In case of majority spin carriers, the valence band (VB) and conduction band (CB) overlap with each other near the Fermi level region, which clearly shows its metallic nature with respective potentials. Similarly, in the case of minority spin carriers, the maxima value of valence band and minima value of conduction band show no band gap in the vicinity of the Fermi level as there is overlapping between these two bands which shows the metallic nature of the compound using GGA and GGA+U. The metallic nature of Pd_2MnSb type structure in spin up channel along with metallic nature in spin down channel predict the full metallic ferromagnetic nature of compound.

To give a clearer image of band structure we have calculated the total density of states (TDOS) with all concerted potentials as shown in Figs. 4 and 5. Through the total density of state, we can explain the energy contribution of all states. In case of TDOS, both major-

Table 2 Magnetic properties of Pd2MnSb compound with GGA and GGA+U respectively

Compound	m^{Inst}	m^{Mn}	m^{sb}	m^{Pd}	m^{c}
Pd_2MnSb (GGA+U)	0.083	4.2	-0.02500	0.15	4.408
Pd_2MnSb (GGA)	0.0811	4.1	-0.02600	0.17218	4.33
Exp[a].					4.40[a]

[a]Ref. (Webster and Ramadan 1977)

ity and minority spin carriers show good agreement with previous results of band structure graphs. The TDOS (Gökoğlu 2012; Hao et al. 2020) plots confirm the full metallic characteristics with GGA and GGA+U potentials: no energy gap appears in both majority and minority spin channels of DOS. Our calculated result from DOS of Pd_2MnSb has similar agreement with band gap properties of Pd_2MnSb. This metallic nature increases the flow of spin polarized current, which leads to high spin polarization ratio in the compound, which is widely used in ferromagnetic materials.

In addition, the interstitial site and individual (Mn, Pd) atoms encourage the overall net moment, whereas the Sb site opposes it, based on the measured values of Pd_2MnSb compound magnetic moment by both potentials, as shown in Figs. 4 and 5. This is because Mn/Pd-d and Sb-p states emerge most frequently over the noted energy range. The antiferromagnetic interaction in between valence band electrons is seen by the opposing sign appearing in the magnetic moments of the Inst, Mn/Pd, whole cell, and Sb elements.

The magnetic properties can be well understood by calculating the partial density of state (PDOS). The asymmetric nature of up and down spins DOS indicates its magnetic nature. As, in the contribution of individual orbitals of Mn, Sb and Pd can clearly observed via partial DOS, orbitals of Mn, Pd and Sb atoms which have contributed dominantly. The P orbital of atom cross the fermi level in the spin up channel resulting its metallic character of compound. Around the Fermi level the higher peak is due to d-orbital is of Mn and Sb among all. From these calculations, we concluded that p orbitals of Pd and d-orbitals of Mn and Sb has more contribution in the band, DOS, and magnetic moment of Pd_2MnSb.

3.3 Magnetic properties

We have studied the magnetic properties (Özdemir et al. 2022; Zada et al. 2022a, b, c; Siddique et al. 2021) of Pd_2MnSb compound by using the graphs of DOS and PDOS. We have calculated the magnetic moment of Pd, Mn and Sb separately by using GGA and GGA+U potential. The value of magnetic moment shows the magnetic characteristics (Bensaid et al. 2016; Zada et al. 2021) of Pd_2MnSb. The interstitial magnetic moment of Pd_2MnSb is also calculated. Table 2 compiles the total magnetic moment, interstitial magnetic moment of Pd_2MnSb and also individual magnetic moment of each atom (Pd, Mn and Sb) with GGA and GGA+U potentials respectively. The total calculated magnetic moment of Pd_2MnSb compound is 4.33 and 4.408 with GGA and GGA+U potentials is close in comparison with experimental measurement. It can be seen that, the Pd_2MnSb has strong magnetic moment and shows ferromagnetic characteristics (Khan et al. 2019; Bibi et al. 2021). The magnetic moment value of Mn atom is high as compared to other atoms like Sb and Pd. Furthermore, the absolute magnetic moment is largely consisting of Mn atom with little addition of Pd atom and interstitial site. The negative value of magnetic moment of antimony (Sb) atom revealed diamagnetic behaviour at all sites in the unit cell shows anti-parallel increment to the entire ferromagnetic direction (Khan et al. 2022a, b, c, d). In consequences, Sb atom definitely effect the ferromagnetic behavior of Pd_2MnSb compound. Moreover, the calculated interstitial site, Mn atom along with entire Pd_2MnSb compound magnetic moment values uplift the ferromagnetic nature, while Sb site opposes it (Khan et al. 2022a, b, c, d). The existence of opposite sign between the magnetic moment of interstitial site, Mn, Sb and Pd atoms along with total magnetic moment of Pd_2MnSb compound using GGA and GGA+U potentials shows valence band electrons associated in anti-parallel behavior (Zada

et al. 2022a, b, c) to the total magnetic moment of compound. Ultimately, the net magnetic moment reveals that Pd_2MnSb compound has strong magnetic nature.

4 Conclusion

In this research work, DFT calculations are performed by using different approximations (PBE-GGA and GGA+U) to study the structural, electronic, and magnetic properties of Pd_2MnSb Heusler compound. The calculated parameters like lattice constants and the stable structure optimization in the FM phase are reliable with other experimental reported results. We study the structural properties and find that the compound Pd_2MnSb has cubic structure. Further, we calculated electronic properties with GGA and GGA+U potentials which show its metallic behavior with both potentials. We calculated the partial density of state to see the particular contribution of different states. The main property of interest is their capability to reach high magnetization levels when subjected to an external magnetic field having metallic characteristics and strong magnetic moment of our selected Heusler alloy Pd_2MnSb. The magnetic moment of Pd_2MnSb is 4.33 and 4.408 with GGA and GGA+U potentials show ferromagnetic material characteristics in nature and widely used in more advanced magnetic storage devices.

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Author contributions Abdul Munam Khan: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Visualization, Writing – original draft; Abdul Ahad Khan: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – review & editing; Zeshan Zada: Conceptualization, Data curation, Formal analysis, Supervision, Validation, Visualization, Methodology, Resources, Software, Writing – review & editing; Ali H. Reshak: Formal analysis, Validation, Visualization Investigation, Methodology, Writing – review & editing; Shakeel: Conceptualization, Resources, Validation, Visualization, Writing – review & editing; Dania Ali: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Validation, Visualization; Muhammad Ismail: Formal analysis, Investigation, Methodology, Validation, Visualization; Muhammad M. Ramli: Formal analysis, Investigation, Methodology.

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Declarations

Competing interests The authors declare no competing interests.

Conflict of interest The author declares no conflict of interests.

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