The Ground-State Properties of a New Full-Heusler Alloy Pd₂MnPb: DFT+U, QTAIM, and MFA Investigations

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1. Introduction

Full-Heusler alloys, named after the German engineer Friedrich Heusler [1], have attracted the attention of researchers because of their magnetic and electronic behaviors. Several theoretical and experimental researchers have found that these compounds have physical properties that can be exploited in several fields of application and several industries. Indeed, these compounds are coveted because of their very varied properties such as their ferromagnetic and antiferromagnetic behaviors, metallic character and their rigidities, etc. [2–7].

This family of materials is used in several technical applications such as magnetic devices [8], spin filters [9], optical properties [10], electrical junctions [11] and giant magneto-resistance devices [12, 13] due to their strong magnetic behaviors compared to other compounds of similar structures [2]. The chemical formula of full-Heusler compounds is X₂YZ, from which, in most of those synthesized, X and Y are generally magnetic elements that belong to transition metals, actinides or lanthanides, while Z is nonmagnetic [14]. The presence of these magnetic elements is the origin of the strong magnetic behaviors of these compounds, most of which are ferromagnetic.

Mn-based full-Heusler compounds (X₂MnZ) belong to this family of materials that are of great importance, the fact which has motivated researchers to determine their properties. Akriche et al. [15] have carried out a complementary study on the elastic, electronic and magnetic properties of Co₂MnGe. They have estimated its Curie temperature and have studied its elastic behavior under the effect of the hydrostatic pressure. Using experimental techniques and first-principles calculations, Ahmed et al. [16] have studied the influence of antisite disorder occupancies on the magnetic properties of Co₂MnSi. They have found almost equal amount of Mn and Co disorder using neutron diffraction studies. They have also found that these latter results are in a good agreement with those obtained by density functional theory (DFT).

Pd₂MnZ-Heusler alloys have very fascinating electronic and magnetic properties because of their ferromagnetic or antiferromagnetic behaviors as well as their

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metallic nature. Their magnetic moments are mainly due to the partial contribution of Mn-atom, which is generally close to 4 $\mu_B$ [17, 18].

DFT based methods, particularly those of the first principles, have largely contributed in the proposition of new compounds by theoretical predictions of their physical behaviors. In this respect, experimenters look for their synthesis because they were fascinated by the results predicted by DFT. In our work, we propose a new compound that is $\text{Pd}_2\text{MnPb}$-Heusler starting with the study of its most stable magnetic ordering and the verification of its energy and mechanical stabilities before moving on to the study of its elastic anisotropy and its electronic and magnetic properties.

2. Computational details

Most of results of this work have been obtained by FPLAPW+lo method [19, 20] which is implemented in WIEN2k code [21, 22]. For this method, and to ensure a good accuracy of results in a reasonable time, the choice of input parameters is of great importance. The crystal structure of $\text{Pd}_2\text{MnPb}$ has been introduced by the atomic positions of the different atoms and the choice of the space group #225.

In Fig. 1 using XCrySDen software [23], we represent respectively the unit-cell and the conventional one of $\text{Pd}_2\text{MnPb}$ in its full-Heusler structure. The initialization of the FPLAPW+lo-based calculations first begins with a choice of $R_{MT}$ from which the values: 2.1, 2.0, and 22 are respectively chosen for Pd, Mn and Pb atoms. GGA-PBE was chosen for the exchange-correlation functional [24]. To ensure a consistent number of plane waves, a value of $R_{K_{\text{max}}}=8.5$ was used. $l_{\text{max}}=10$ and $G_{\text{max}}=12$ were taken for the maximum value of the partial waves inside atomic spheres and for the largest value of $G$ vector for the Fourier expansion charge. In this work, the choice of $k$-mesh of the irreducible Brillouin zone (IBZ) [25] is 1500 $k$-points for the nonmagnetic order, 3000 $k$-points for the ferromagnetic order and 800 $k$-points for the antiferromagnetic one. All results have been adopted by a convergence of the total energy with a limit value of $10^{-5}$ Ry.

In this work, other methods have also been used for the prediction of other physical properties such as the quantum theory of atoms in molecules method (QTAIM) [26, 27], which is implemented in Croton code [28, 29] for determining the positions of bonds and spin polarized relativistic Korringa–Kohn–Rostoker method, which is implemented in SPR-KKR package [30, 31], to calculate the exchange coupling parameters $J_{ij}$ for the estimation of the Curie temperature of $\text{Pd}_2\text{MnPb}$ using mean field approximation (MFA) [32, 33].

For QTAIM method, calculations are based on the results of the total electron density that is obtained by FPLAPW+lo. For a good accuracy of the results and to determine the different critical points (more detail are introduced in the electronic part) for $\text{Pd}_2\text{MnPb}$ in its most stable magnetic ordering (ferromagnetic) the $k$-points number has been increased up to 10000.

For SPR-KKR method, the full-potential spin-polarized scalar relativistic approach was used. For the angular momentum cutoff, a maximum value $l_{\text{max}}=4$ was chosen. 750 $k$-points were used for the mesh of the irreducible Brillouin zone (IBZ). A value of $10^{-5}$ eV has been adopted as a limit for the convergence of the total energy.

3. Results and discussions

3.1. Most stable magnetic ordering and structural properties

In order to propose a new compound that is not yet synthesized, it is important to determine, in a first time, its structural parameters and its most stable magnetic ordering. Fitting the curve of variation of the total energy as a function of the unit-cell (or conventional-cell) volume $E=F(V)$ by one of the equations of states (EOS) allows the determination of several structural parameters, in particular the lattice parameter, bulk modulus and its pressure derivative. This study also allows the determination of the most stable magnetic ordering focusing on the comparison between the curves of these variations in several magnetic orders (nonmagnetic NM, ferromagnetic FM and antiferromagnetic AFM) from which the most stable order is that which has the minima of the total energy compared with the minima of the other magnetic orders variations.

Figure 2 shows $E=F(V)$ variations in the different magnetic ordering, from which we can notice that FM order is the most stable, leading to that $\text{Pd}_2\text{MnPb}$ is ferromagnetic. It confirms, therefore, what was mentioned in the introduction that this kind of compounds have a strong magnetic behavior. On the other hand, the different $E=F(V)$ curves have been fitted with Murnaghan equation [34], and the obtained structural results are grouped in Table I. We notice that the total energy of the unit-cell of FM ordering is the lowest which confirms the ferromagnetic behavior of this compound.
The Ground-State Properties of a New Full-Heusler Alloy $\text{Pd}_2\text{MnPb}$. . .

Fig. 2. Variations of the total energy as a function of volume of $\text{Pd}_2\text{MnPb}$ in nonmagnetic, antiferromagnetic and ferromagnetic orderings.

TABLE I

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>$a_0$ [Å]</th>
<th>$B_0$ [GPa]</th>
<th>$B'$</th>
<th>$E_0$ [eV/atom]</th>
<th>$E_{\text{coh}}$ [eV/atom]</th>
</tr>
</thead>
<tbody>
<tr>
<td>NM</td>
<td>6.4235</td>
<td>140.6189</td>
<td>5.2282</td>
<td>$-87533.01080$</td>
<td>$-11.4057$</td>
</tr>
<tr>
<td>AFM</td>
<td>6.5562</td>
<td>105.7514</td>
<td>5.8997</td>
<td>$-87533.13531$</td>
<td>$-12.7173$</td>
</tr>
</tbody>
</table>

On the other hand, we note that the values of the lattice parameter and the bulk modulus of FM and AFM orders are similar and far from those obtained for NM one, which confirms the magnetic behavior of this compound. The magnetic behavior of this compound as well as its energy stability can be confirmed by the determination of the cohesive energy. Where, for this compound, its expression is given as the following:

$$E_{\text{Coh}}^{\text{Pd}_2\text{MnPb}} = E_{\text{total}}^{\text{Pd}_2\text{MnPb}} - (2E_{\text{atom}}^{\text{Pd}} + E_{\text{atom}}^{\text{Mn}} + E_{\text{atom}}^{\text{Pb}}).$$

The estimation of $C_{11} + 2C_{12}$, $C_{11} - C_{12}$ and $C_{44}$ by the three distortions $D_i$ is realized through the pairing between the polynomial fits of the unit-cell energy variations as a function of the applied strain $E_{D_i}(\delta)$ and the theoretical equations of these variations according to the theoretical used model, which are given respectively by [38, 39]:

$$E_{D_1}(\delta) = E_0 + V_0(\delta_{\text{str}}) + O(\delta^2),$$

$$E_{D_2}(\delta) = E_0 + V_0(\delta_{\text{str}} + O(\delta^2)),$$

$$E_{D_3}(\delta) = E_0 + V_0(2C_{44}\delta + O(\delta^2)).$$

It has already been mentioned that $\text{Pd}_2\text{MnPb}$ full-Heusler has not been synthesized yet. On the other hand, it has been predicted in the structural part that this compound is energetically stable. In this section, we will check its mechanical stability and its elastic behavior as well as its elastic anisotropy. We recall that a compound of cubic structure has three elastic constants noted $C_{11}$, $C_{12}$ and $C_{44}$. In this respect, for being mechanically stable it is necessary that their values respond to the Born criteria of mechanical stability which are given by the following expressions [35–37]:

$$C_{11} + 2C_{12} > 0, \quad C_{11} - C_{12} > 0 \quad \text{and} \quad C_{44} > 0.$$
realized by the following expression [43–48]:

\[ \theta_D = \frac{h}{k_B} \left( \frac{3n N_A M}{4\pi R} \right)^{1/3} V_a, \]

whereby: \( n, M, h, k_B, \rho, N_A \) and \( V_a \) represent respectively the number of atoms per unit cell, molecular mass, Planck’s constant, Boltzmann’s constant, the density, Avogadro constant and the average elastic wave velocity. The latter physical quantity \( V_a \) is based on the knowledge of the mechanical quantities related to the elastic constants [43–48], from which for its estimation, their Hill’s average values have been used. The obtained value of the Debye temperature is shown in Table II.

### 3.3. Elastic anisotropy

The confirmation of the mechanical stability of this compound allows studying its elastic anisotropy and better understanding its elastic behavior according to the different directions of space. Generally, we can know if a compound is elastically isotropic or anisotropic by analyzing the value of the universal elastic anisotropy index \( A^U \) which is given by the following expression [49]:

\[ A^U = \frac{5G_V}{G_R} + \frac{B_V}{B_R} - 6. \]

This index is mainly based on the difference between the bulk modulus values and those of the shear modulus which are obtained by the two approximations: that of Reuss and that of Voigt. It can be predicted that a compound is elastically isotropic in case if the value of this index is close or equal to zero. Otherwise it is elastically anisotropic for any value far from zero. We also note that the more the value of this index is far from zero, the more the elastic anisotropy is large. From Table II, \( A^U \) found value is very far from zero indicating that Pd\(_2\)MnPb, in its full-Heusler structure, has a very wide elastic anisotropy.

This index can inform us about the elastic isotropy/anisotropy of Pd\(_2\)MnPb but it does not allow us to study this behavior according to the three directions of space. For a better understanding of the origin of this large elastic anisotropy and to determine the directions for which this anisotropy is large or small, we have studied the anisotropy of Young’s modulus based on the approach proposed by Nye [50]. According to this theoretical approach, for a cubic structure, the variation of Young’s modulus according to the three directions of space obeys the following equation [50]:

\[ E = \frac{1}{S_{11} - 2 \left( S_{11} - S_{12} - \frac{1}{2} S_{44} \right) \left( I_1 I_2^2 + I_2 I_3^2 + I_3 I_1^2 \right)}. \]

This equation is based on the elastic compliance constants \( S_{ij} \) and the direction cosines \( i_i \). Knowing the values of Young’s modulus along the three directions of space, this variation can be represented as a closed surface. By analyzing the shape of this surface, we can predict whether the material is elastically isotropic or anisotropic. Hence for an isotropic compound, the value of Young’s modulus is invariable in the three directions of space, which gives a surface of a sphere of \( E \) radius.

### Table II

<table>
<thead>
<tr>
<th>( C_{11} ) [GPa]</th>
<th>( G_H )</th>
<th>( E_V )</th>
<th>( \theta_D )</th>
<th>( A_u )</th>
<th>( E_a )</th>
</tr>
</thead>
<tbody>
<tr>
<td>107.9406</td>
<td>54.958</td>
<td>86.958</td>
<td>179.528</td>
<td>9.6310</td>
<td>36.3934</td>
</tr>
<tr>
<td>97.8557</td>
<td>31.709</td>
<td>60.229</td>
<td>128.8670</td>
<td>14.8802</td>
<td></td>
</tr>
<tr>
<td>50.0489</td>
<td>60.229</td>
<td>101.217</td>
<td>14.8802</td>
<td>36.9384</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 3. Variations of the total energy as a function of the applied strains according to the different distortions for Pd\(_2\)MnPb.

**TABLE II**

Calculated elastic constants \( C_{ij} \) [GPa], Voigt, Reuss and Hill values of: shear modulus \( G \) [GPa], Young’s modulus \( E \) [GPa] and Bulk modulus \( B \) [GPa]. The universal elastic anisotropy index \( A^U \), Debye temperature \( \theta_D \) [K], maximum, minimum and average values of Young’s modulus \( E_{\text{max}}, E_{\text{min}} \) and \( E_a \) [GPa] of Pd\(_2\)MnPb.

\[ B_R = B_V = B_H = \frac{C_{11} + 2C_{12}}{3}, \]

\[ G_R = \frac{5C_{44}(C_{11} - C_{12})}{3(C_{11} - C_{12}) + 4C_{44}}, \]

\[ G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5}, \]

\[ E_{R,V,H} = \frac{9G_R V_R B}{G_{R,V,H} + 3B}. \]

Their obtained values are grouped in Table II from which we can deduce that the obtained value for the bulk modulus is very close to that found in the structural part which confirms the precision of this theoretical model and our results. Furthermore for Young’s modulus or shear modulus, we notice a very large difference between the value obtained by the Reuss approximation and that obtained by the Voigt approximation, which indicates that this compound has a large elastic anisotropy that will be dealt with in detail in the next section of this work.

The knowledge of the elastic constants and their related mechanical quantities allows the determination of the Debye temperature. This thermodynamic quantity is related to the vibrations of Pd\(_2\)MnPb atoms because it represents the temperature for which the maximum vibration normal mode is reached. Its determination is realized by the following expression [43–48]:

\[ \theta_D = \frac{h}{k_B} \left( \frac{3n N_A M}{4\pi R} \right)^{1/3} V_a, \]
Contrary to that if Young’s modulus is variable, the surface will be deformed and the more it is deformed compared to the spherical form, the more the elastic anisotropy is large.

In Fig. 4 we have plotted the directional dependence surface of Young’s modulus of Pd$_2$MnPb. It can be clearly observed that it is very deformed with respect to a spherical surface which indicates that this compound has a very large elastic anisotropy. This confirms our result obtained by the universal elastic anisotropy index. According to this surface, and according to Table II, the maximum value of Young’s modulus $E_{\text{max}}$ is very different from that minimal $E_{\text{min}}$ because of the large anisotropy of this compound and the average value along this whole surface $E_{\text{a}}$ is very close to that obtained by the Reuss approximation, which confirms the precision of this theoretical model.

To better understand the directions for which the elastic anisotropy is large or small, the directional dependence surface of Young’s modulus has been projected according to the most critical planes; (001), (110) and (111) (as shown in Fig. 5). It can be seen that the minimum value is according to (001) and (110) planes, while the maximum value is according to (110) plane. In addition, it should be stated that the directional dependence surface of Young’s modulus is too deformed according to (110) plane, which indicates that according to this plane the elastic anisotropy is too large, while this surface is less deformed according to (111) plane, which indicates that the elastic anisotropy is less large according to this plane, but the surface according to this last plane is still far from being circular which indicates that despite of being less deformed, the elastic anisotropy remains always large.

3.4. Electronic and magnetic properties

In the previous sections of this work, we have shown that Pd$_2$MnPb is mechanically stable in its ferromagnetic ordering. This allowed us to also determine its electronic and magnetic behaviors by studying its electronic band structure and by analyzing the curves of total and partial densities of states. We recall that Pd$_2$MnPb contains a Mn-atom which has strongly correlated 3d electrons. Semilocal functionals do not take into account this strong correlation and give generally erroneous electronic behaviors for this kind of materials [51]. For our compound, and in order to solve this problem, a correction has been added to GGA functional used in this work. This correction is represented by the effective on-site Coulomb interaction parameter $U_{\text{eff}}$ (Hubbard’s correction) [51]. We have estimated its value by constrained LDA method cLDA described in several previous works [52–54] using the following equation:

$$U_{\text{eff}} = E_{\text{Mn 3d}^\uparrow}(+\frac{1}{2}e) - E_{\text{Mn 3d}^\uparrow}(-\frac{1}{2}e) - E_{\text{F}}(+\frac{1}{2}e) + E_{\text{F}}(-\frac{1}{2}e).$$ (13)

The obtained values of the effective on-site Coulomb interaction parameter $U_{\text{eff}}$, the spin-up eigenvalues of Mn 3d states “$E_{\text{Mn 3d}^\uparrow}$” as well as those of the Fermi energies related to the addition and the removal of Mn 3d electrons are grouped in Table III.

Using GGA and GGA+U, we have obtained the two electronic band structures of Pd$_2$MnPb that are represented in Figs. 6 and 7 in parallel with the curves of the partial densities of states. We can see from these figures that Hubbard’s correction has shifted the spin down peaks of Mn d states of the conduction band to a higher energy level and it has shifted the spin up peaks of Mn d and Pd d of the valence band to a lower energy level with a large change in the shape of the peaks. Despite this correction, it can be seen that there is always an overlap of the bands between the valence band top and the conduction band bottom which shows that this compound is a metal. These figures show that the valence band top and the conduction band bottom are mainly dominated by Mn d and Pd d states. In addition, the great difference
Calculated spin-up eigenvalues of Mn 3d states \( E_{\text{Mn 3d}} \) [eV] and Fermi energies \( E_F \) [eV] corresponding to addition and removal of electrons. The effective on-site Coulomb interaction parameter \( U_{\text{eff}} \) [eV], Curie temperature \( T_C \) [K], total and partial magnetic moments \([\mu_B]\) and spin polarization \(P\%\) of Pd\(_2\)MnPb.

<table>
<thead>
<tr>
<th></th>
<th>( E_{\text{Mn 3d}} ) (+0.5e)</th>
<th>( E_{\text{Mn 3d}} ) (-0.5e)</th>
<th>( E_F ) (+0.5e)</th>
<th>( E_F ) (-0.5e)</th>
<th>( U_{\text{eff}} )</th>
<th>( T_C )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Magnetic moment</td>
<td>Pd</td>
<td>Mn</td>
<td>Pb</td>
<td>Total</td>
<td>Interstitial</td>
<td>P</td>
</tr>
<tr>
<td>GGA</td>
<td>0.10337</td>
<td>3.81655</td>
<td>-0.00582</td>
<td>4.32972</td>
<td>0.31223</td>
<td>8.17</td>
</tr>
<tr>
<td>GGA+U</td>
<td>0.07439</td>
<td>4.28381</td>
<td>0.00749</td>
<td>4.77921</td>
<td>0.33913</td>
<td>-13.53</td>
</tr>
</tbody>
</table>

Fig. 6. Calculated spin-up electronic band structures and the partial densities of states using GGA (solid lines) and GGA+U (dashed lines) for Pd\(_2\)MnPb.

between the peaks of the both spins shows the strong ferromagnetic behavior of this compound. To confirm this, the spin polarization \(P\) has been calculated using GGA and GGA+U using the following expression [40]:

\[
P = \frac{\rho^\uparrow(\varepsilon_F) - \rho^\downarrow(\varepsilon_F)}{\rho^\uparrow(\varepsilon_F) + \rho^\downarrow(\varepsilon_F)},
\]

where \(\rho^\uparrow(\varepsilon_F)\) and \(\rho^\downarrow(\varepsilon_F)\) represent respectively the total density of states near the Fermi level for both spins.

From Table III, the spin polarization values obtained by GGA and GGA+U are different from zero and 100%, which confirms the metallic and ferromagnetic natures of Pd\(_2\)MnPb. Table III also contains the values of the total, interstitial and partial magnetic moments that have been obtained by GGA and GGA+U, from which it can be stated that the total magnetic moment is large because of the strong ferromagnetic nature of this compound. Furthermore, the great contribution is that of the magnetic moment of Mn-atom, which is about 4 \(\mu_B\) which also confirms what has already been mentioned in the introduction.

3.5. Estimation of Curie temperature

The most stable magnetic ordering of Pd\(_2\)MnPb in its full-Heusler structure has already been determined from which it has been found that it is a ferromagnetic compound. In this section, we have estimated its Curie temperature by mean field approximation (MFA) method [32, 33] using the following equation:

\[
\frac{3}{2}k_B T_C^{\text{MFA}} = J^0_{\mu\nu},
\]

in which \(k_B\) and \(J^0_{\mu\nu}\) represent respectively the Boltzmann constant and the largest eigenvalue of the matrix of the exchange coupling parameters \(J_{ij}\) between the different atoms of Pd\(_2\)MnPb. As a result, the calculation of the exchange coupling parameters \(J_{ij}\) is primordial.

In this work, the exchange coupling parameters \(J_{ij}\) have been determined by the spin system Hamiltonian of the classical Heisenberg model using spin polarized relativistic Korkina–Kohn–Rostoker (SPR-KKR) code [30, 31]. This latter method makes it possible to calculate the different exchange coupling parameters \(J_{ij}\) between the different atoms and also makes it possible to confirm the most stable magnetic ordering of the studied compound.

Figure 8 represents the variation of exchange coupling parameters \(J_{ij}\) according to the cluster distance, which is centered by Mn atom. It is clearly seen that the Mn–Mn interaction between the two nearest-neighbors is the most dominant and has a positive sign. The second Mn–Mn interaction is also positive and the sum of all Mn–Mn interactions is also positive, which confirms that this compound has a ferromagnetic behavior.
The other interactions between Mn and the other atoms are relatively small contributors in comparison with that of Mn–Mn. On the other hand, all the interactions become negligible for a distance of around 2.5a, which confirms that the maximum chosen distance of the cluster is largely sufficient. Using Eq. (15) and the values of the exchange coupling parameters that we have determined, the Curie temperature of Pd$_2$MnPb, in its full-Heusler structure, has been estimated (Table III).

3.6. Bonding analysis

The prediction of the bonding types between the atoms that form Pd$_2$MnPb is one of the main objectives of this work. To determine the different positions and the number of bonds between the different atoms that form Pd$_2$MnPb, the QTAIM has been used, while their natures have been predicted by calculating the ionicity factor. QTAIM approach is mainly based on the topological analysis of the electron density in a molecule or a crystal as in our case [26, 27]. According to this approach (QTAIM), the atoms are considered as electron basins separated by surfaces on which the flux of the gradient vector field of the electron density is zero (the projection of these surfaces according to (110) plane is shown by dark lines in Fig. 9). All these characteristics are based on the determination of the critical points CPs of the spatial distribution of the electronic density which are characterized by a zero gradient vector field of the electron density. According to a given direction, the critical point is the position of maximum/minimum of the electronic density and according to this basis that the critical points are classified (bond, cage and ring critical points). What interests us among all these points is the one of the bond (BCP) because it permits to show the presence of the different bonds between the different atoms and consequently, the determination of their numbers and their positions. BCP is the point of the zero flux surfaces, which separates the bounded atoms, where a single gradient path ($\nabla \rho(r)$ trajectory) starting from the nucleus meets another identical path of the other neighboring atom. Figure 9 shows the gradient vector paths of the electronic density that start from the nuclei and reach the zero flux surfaces along the densest plane (110). The different bond critical points (BCPs) are indicated by a B letter. According to this figure, it can be mentioned that the bonds which exist between the different atoms that form Pd$_2$MnPb are: Pb–Pd, P–Pd, P–Mn and Mn–Pb. The positions of the different BCPs are shown in Table IV. This table also contains the values of the ionicity factor based on Pauling electronegativities [55] which makes it possible to predict the behavior of a bond between two atoms A and B. Its expression is given by

$$\text{IF}_{A-B} = 1 - \exp \left( - \frac{(\chi_A - \chi_B)^2}{4} \right).$$

(16)

$\chi_A$ and $\chi_B$ represent respectively the values of Pauling electronegativities of A atom and B atom. A value close to 1 of this factor indicates that the bond between A and B is of ionic character, while a value close to zero indicates a covalent character. From Table IV, all ionicity factor values for the different bonds are close to zero indicating that all bonds have a strong covalent character.
4. Conclusion

The present work is a first prediction of the most stable magnetic ordering, structural, elastic, electronic and magnetic properties of a new full-Heusler compound Pd₂MnPb using mainly FPLAPW+lo method which is implemented in WIEN2k code. The most remarkable conclusions of each property are listed below:

- The results of the structural properties have shown that the values of the lattice parameter for FM and AFM magnetic orders are similar, while they are far from those obtained for NM order, which indicates the strong magnetic behavior of Pd₂MnPb. The analysis of the minima of $E = F(V)$ curves in the three studied magnetic orders has shown that this compound has a ferromagnetic behavior. The cohesive energy values have confirmed these results and they have shown the energy stability of this compound.

- The study of elastic properties has shown that Pd₂MnPb is mechanically stable. The determination of the elastic constants allows the determination of other mechanical quantities such as Young’s modulus, shear modulus and the Debye temperature. The prediction of the universal elastic anisotropy index and the analysis of the directional dependence surface of Young’s modulus have shown that this compound has a large elastic anisotropy.

- The electronic properties have been determined taking into account the strong correlation between Mn 3d electrons by the estimate of the effective on-site Coulomb interaction parameter $U_{\text{eff}}$, which has been added to GGA functional as a correction. Despite this correction, the obtained results by GGA and GGA+U have shown that Pd₂MnPb has a strong metallic character. The spin polarization values have confirmed its ferromagnetic behavior. The Curie temperature has been estimated by mean-field approximation MFA using the values of the exchange coupling parameters $J_{ij}$ obtained by SPR-KKR method. The results of the latter have confirmed the ferromagnetic character of this compound. The analyses of the bonds between the atoms that form Pd₂MnPb using QTAIM and the values of the ionicity factor have shown that they have all a strong covalent character.

References

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