Structural, elastic, electronic and thermodynamic properties of uranium filled skutterudites UFe$_4$P$_{12}$: First principle method

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**Abstract**

We present a theoretical study of structural, elastic, thermodynamic, and electronic properties of the uranium filled skutterudite UFe$_4$P$_{12}$. We use the full-potential linear muffin–tin orbital (FP-LMTO) method in which the local density approximation (LDA) is used for the exchange-correlation (XC) potential. The lattice parameter at equilibrium, the bulk modulus, its pressure derivative, the elastic constants and the band structure energy of the filled skutterudite UFe$_4$P$_{12}$ are calculated and systematically compared to available theoretical and experimental data. Herein, we use the total energy variation as function of strain technique to determine independent elastic constants and their pressure dependence. Furthermore, using quasi-harmonic Debye model with phonon effects, the effect of pressure $P$ and temperature $T$ on the lattice parameter, bulk modulus, thermal expansion coefficient, Debye temperature and the heat capacity of UFe$_4$P$_{12}$ are investigated for the first time. Band structure of UFe$_4$P$_{12}$ indicates a tendency of forming a pseudo-gap that appears above the Fermi level at $\Gamma$ point. This is a unique characteristic of skutterudite, especially when a single phosphorous p-band crosses the Fermi level. The crossing band is, indeed, pushed down by the repulsion of U-f-resonance states.

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1. **Introduction**

The family of filled skutterudites usually crystallizes in cubic structure with space group Im$\bar{3}$ [1,2]. These are generally described by MT$_4$X$_{12}$ formula (M=rare earth, T=Fe, Ru, Os; X=P, As, Sb). The uranium filled skutterudites have been a subject of unprecedented research in the recent past due to properties as these are characterized by large thermoelectric potential [3], these show traces of superconductivity [4,5], small hybridization gap semiconductivity [6,7], valence fluctuation [6,8–10], heavy Fermionic behavior [8–11], non-Fermi liquid behavior [12,13], and magnetic characteristics [7,14].

The physical properties of the filled skutterudites compound depend on M atom hybridization between the f-electron states of M atom with the conduction electron...
states. In particular, UFe₄P₁₂ is the subject of immense interest. The structural properties of UFe₄P₁₂ filled skutterdites are determined using the neutron diffraction technique [15]. It is noticed that UFe₄P₁₂ is ferromagnetic at Curie temperature of 3.1 K. The optical properties have been probed experimentally and it is noticed that hybridization has a major role to determining the properties of MFe₄P₁₂ [16]. The electronic structure of YbFe₄P₁₂, UFe₄P₁₂ and ThFe₄P₁₂ is studied using tight-binding approach, which shows that YbFe₄P₁₂ and UFe₄P₁₂ exhibit half metallic behavior, however ThFe₄P₁₂ compound is metallic nature [17]. The magnetic response, the effect of high magnetic field and specific heat of single crystals are reported [18]. A coupling between 5f electron and ³¹P nuclei is substantial in UFe₄P₁₂ than PrFe₄P₁₂ [19].

Motivated from the earlier reported studies on uranium filled skutterdite, we aim at studying the structural, elastic, electronic and thermodynamic properties using first principle method and following full-potential linear muffin–tin orbital (FP-LMTO) method within local density approximation (LDA) using exchange-correlation (XC) potential. The present paper is organized as follows: Section 2 briefly discusses the computational method used in calculations; while Section 3 is concerned with deduced results and their discussions. A comparison is also made with the available investigations.

2. Computational details

The calculations presented in this paper on UFe₄P₁₂ compound are carried out using the full-potential linear muffin–tin–orbital (FP-LMTO) method [20,21] as implemented in Lmto code [22]. However, the exchange-correlation potential are described within local density approximation (LDA) using the scheme developed by Perdew–Wang [23,24]. The space, which is considered by this calculations method, is divided into two parts: an interstitial region (IR) and non-overlapping (MT) spheres centered at the atomic sites. Furthermore, in the (IR) region the basic functions are illustrated in terms of Fourier series. Inside the (MT) spheres, the basic sets are described principally by radial solutions of the one-particle Schrödinger equation (at fixed energy) and their energy derivatives multiplied by harmonical spheres.

The valence wave functions inside the spheres are expanded up to \( l_{\text{max}} = 6 \). The integrals over the Brillouin zone are performed up to \( 6 \times 6 \times 6 \) grid using the Bloch’s modified tetrahedron method [25]. The self-consistent calculations are converged only, when the total energy converges to less than \( 10^{-6} \) Ry. The \( k \) integration over the Brillouin zone is performed on method using the tetrahedron method [26]. Values of sphere radius (MTS) taken for each atomic position, energy cut-off for filled skutterdites UFe₄P₁₂ and the number of plane waves used in the present calculations are listed in Table 1.

3. Results and discussion

3.1. Equilibrium lattice and bulk modulus

The schematic diagram of crystal structure used here is documented in Fig. 1. The U, Fe and P atoms are positioned respectively as follows: \((0, 0, 0)\), \((-1/4, 1/4, 1/4)\), \((1/4, -1/4, 1/4)\), \((1/4, 1/4, -1/4)\) for Fe and P atoms located at \((0, y, z)\), \((0, y, -z)\), \((z, 0, y)\), \((-z, 0, y)\), \((y, z, 0)\), \((y, -z, 0)\), \((0, -y, -z)\), \((0, -y, z)\), \((-z, 0, -y)\), \((z, 0, -y)\), \((-y, -z, 0)\), \((-y, z, 0)\). We performed structural optimization by minimizing the total energy with respect to atomic positions \( y \) and \( z \) and the lattice parameters.

While estimating the ground state properties of UFe₄P₁₂, the total energies are calculated for different volumes around the equilibrium cell volume. In Fig. 2, we present the variation of the total energy as function of cell volume. Calculated total energy was fitted to Murnaghan’s equation of state [27]. We, thus, determine the lattice constant \( a_0 \), the bulk modulus \( B_0 \) and its pressure derivative \( X \) and \( Y \), which are summarized in Table 2 together with available experimental and theoretical values.

We note that LDA calculations yield the equilibrium lattice parameter \( a_0 \) (7.651 Å) consistent with the neutron-diffraction data [15]. It is worth to comment that variation in \( a_0 \) as compared to neutron-diffraction data (\( T = 15 \) K) is attributed to temperature effect. We further determine bulk modulus and the pressure derivative of UFe₄P₁₂ and their values are documented in Table 2. Due to the lack of experimental and theoretical data, a comparison could not be made and hence these are predictive studies for future investigations.

<table>
<thead>
<tr>
<th>Atom</th>
<th>U</th>
<th>Fe</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ecut-off (Ry)</td>
<td>137.0767</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MTS (a.u.)</td>
<td>3.97</td>
<td>2.39</td>
<td>2.49</td>
</tr>
</tbody>
</table>
3.2. Elastic properties

The elastic properties provide information about capability of materials deformation under applied external forces. Therefore, the stability, stiffness and structural phase of materials changes. For a cubic crystal, there are three independent second-order elastic constants, namely $C_{11}$, $C_{12}$, and $C_{44}$ [28]. The determination of elastic constants needs to know nature of strain, and orthorhombic strain conserving volume is used to calculate $C_{11} - C_{12}$ and $C_{44}$. For identification of $C_{44}$, we used a monoclinic strain conserving volume defined as

$$
\tau = \begin{bmatrix}
\delta & 0 & 0 \\
0 & \delta & 0 \\
0 & 0 & \frac{1}{(1+\delta^2)} - 1 
\end{bmatrix}
$$

(1)

The energy total is influenced by the application of this strain and is expressed as

$$
E(\delta) = E(0) + 6(C_{11} - C_{12})V_0\delta^2 + O(\delta^4)
$$

(2)

The bulk modulus is

$$
B = (C_{11} + 2C_{12})/3
$$

(3)

For identification of $C_{44}$, we used a monoclinic strain conserving volume defined as

$$
\tau = \begin{bmatrix}
1 & \frac{2}{\delta} & 0 \\
\frac{2}{\delta} & 1 & 0 \\
0 & 0 & \frac{4}{(1+\delta^2)} 
\end{bmatrix}
$$

(4)

The total energy is thus

$$
E(\delta) = E(0) + \frac{1}{2}C_{44}V_0\delta^2 + O(\delta^4)
$$

(5)

The variation of the total energy with a orthorhombic (a) and monoclinic (b) of stress at different pressure is illustrated in Fig. 3, and is utilized for determination of $C_{11} - C_{12}$ and $C_{44}$. Table 3 lists the calculated elastic constants $C_{11}$, $C_{12}$ and $C_{44}$ in the pressure range from −20 GPa to 50 GPa with steps of 10 GPa. It is noticed that in the cubic crystal, the values of elastic quantities $C_{11}$, $C_{12}$ and $C_{44}$ validates the condition of mechanical stability [29]: $C_{11} - C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$ and $(C_{11} + 2C_{12}) > 0$.

We note that UFe₄P₁₂ is the mechanical stable in the studied pressure range. In the isotropic system, the anisotropic factor is computed using formula: $A=2C_{44}/(C_{11} - C_{12})$, this factor is a unity in isotropic crystal. The calculated value of anisotropic factor in Table 3 is larger than 1, so UFe₄P₁₂ is anisotropic material in the studied pressure range. Elastic quantities as shear modulus $G$, Young’s modulus $E$, and Poisson’s ratio $\nu$, are derived from elastic constants and are [30–32]

$$
\nu = \frac{3B - E}{6B}
$$

(6)

$$
E = \frac{9BG}{3B+G}
$$

(7)
In Table 3, the value of bulk modulus $B_0$ calculated by expression (3) at $P=0$ GPa is documented. It is noted that calculated value is nearly the same as obtained from fitted Murnaghan’s equation of state. The Poisson’s ratio $\nu$ reflects information about the plasticity of the materials. The lower and upper limit for central force materials are $\nu=0.25$ and $\nu=0.5$, respectively [33–36]. For UFe$_4$P$_{12}$, we deduce Poisson’s ratio lower than 0.25 for the entire pressure range. We can say that the interatomic forces are dominant for UFe$_4$P$_{12}$. In order to determine the nature of the material, Pugh [37] suggested a simple criterion $B/G$; if the value obtained of $B/G > 1.75$ the ductility of the compound is provided. Otherwise, the material is brittle. The values of $B/G$ documented for UFe$_4$P$_{12}$ in Table 3 infers brittle character.

The variation of the elastic constants ($C_{11}$, $C_{12}$, $C_{44}$) and the bulk modulus ($B$) is presented in Fig. 4. It is clear that the elastic constants $C_{ij}$ increase linearly, when the pressure is enhanced. The linear pressure coefficients of elastic constants $\partial C_{11}/\partial P$, $\partial C_{12}/\partial P$, $\partial C_{44}/\partial P$ and $\partial B/\partial P$ are 4.95, 2.99, 2.08 and 3.64, respectively.

$$G = \frac{C_{11} - C_{12} + 3C_{44}}{5} \quad (8)$$
3.3. Thermodynamic properties

Thermodynamic properties of materials are important to study the material characteristics relevant for industrial applications. Moreover, the properties subjected to high-pressure and high-temperature are of great means in disseminating knowledge at conceptual level of materials. While studying, the thermodynamic properties of UFe₄P₁₂, we apply the quasi-harmonic Debye model as implemented in the Gibbs program [38]. The quasi-harmonic Debye model allows us to obtain all thermodynamics quantities from the calculated energy–volume points, in which the non-equilibrium Gibbs function $G(n; V, P, T)$ is expressed as follows:

$$ G(n; V, P, T) = E(V) + PV + A_{\text{vib}}(\theta_D(V); T) $$

(9)

here $E(V)$ is the total energy per unit cell, $PV$ corresponds to the constant hydrostatic pressure condition, $\theta_D(V)$ is the Debye temperature, and $A_{\text{vib}}$ is the vibration Helmholtz free energy. According to quasi-harmonic Debye model of phonon density of states, one writes $A_{\text{vib}}$ as [39]

$$ A_{\text{vib}}(\theta_D, T) = nK_B T \left[ \frac{\hbar^2}{8\pi I} + 3 \ln \left( 1 - e^{-\theta_D/T} \right) - D \left( \frac{\theta_D}{T} \right) \right] $$

(10)

here $n$ is the number of atoms per formula unit, $K_B$ is the Boltzmann’s constant, $D(\theta_D/T)$ represents the Debye integral. For an isotropic solid, $\theta_D$ is expressed as [38,40]

$$ \theta_D = \frac{\hbar}{K_B} \left( \frac{3}{8\pi nV_1^3} \right)^{1/3} f(\sigma) \sqrt{\frac{B_s}{M}} $$

(11)

here $M$ is the molecular mass per unit cell and $B_s$ is the adiabatic bulk modulus measuring the compressibility of crystal, which is approximated by static compressibility as [41]

$$ B_s \approx B(V) = \sqrt{\frac{d^2E(V)}{dV^2}} $$

(12)

Details of quantities $f(\sigma)$ and $B_s$ are given in Refs. [42–44]. Therefore, the non-equilibrium Gibbs function $G^*$ is a function of $(V, P, T)$ and is minimized with respect to volume $V$.

$$ \left[ \frac{\partial G(V, P, T)}{\partial V} \right]_{P, T} = 0 $$

(13)

By solving Eq. (13), we get the thermal equation (EOS) $V(P, T)$. Heat capacity at constant volume $C_V$ and thermal

### Table 3

Calculated elastic constant $C_{11}, C_{12}, C_{44}$ (in GPa), Bulk modulus (in GPa), Young and shear modulus $E, G$ (in GPa), Poisson’s ratio $\nu$, and the anisotropic parameter $A$ for UFe₄P₁₂.

<table>
<thead>
<tr>
<th>$P$ (GPa)</th>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{44}$</th>
<th>$B=(C_{11}+2C_{12})/3$</th>
<th>$G$</th>
<th>$E$</th>
<th>$\nu$</th>
<th>$A$</th>
<th>$B/G$</th>
</tr>
</thead>
<tbody>
<tr>
<td>–20</td>
<td>418.69</td>
<td>–23.78</td>
<td>337.92</td>
<td>123.71</td>
<td>291.25</td>
<td>489.56</td>
<td>–0.16</td>
<td>1.5</td>
<td>0.4</td>
</tr>
<tr>
<td>–10</td>
<td>478.19</td>
<td>6.62</td>
<td>366.77</td>
<td>163.81</td>
<td>314.38</td>
<td>574.5</td>
<td>–0.08</td>
<td>1.55</td>
<td>0.5</td>
</tr>
<tr>
<td>0</td>
<td>524.11</td>
<td>36.787</td>
<td>386.83</td>
<td>198.227</td>
<td>329.56</td>
<td>637.3</td>
<td>–0.03</td>
<td>1.59</td>
<td>0.6</td>
</tr>
<tr>
<td>10</td>
<td>570.76</td>
<td>67.18</td>
<td>392.91</td>
<td>235.04</td>
<td>336.46</td>
<td>683.32</td>
<td>0.014</td>
<td>1.56</td>
<td>0.7</td>
</tr>
<tr>
<td>30</td>
<td>670.07</td>
<td>125.62</td>
<td>423.52</td>
<td>307.1</td>
<td>363.6</td>
<td>781.2</td>
<td>0.076</td>
<td>1.56</td>
<td>0.85</td>
</tr>
<tr>
<td>50</td>
<td>753.52</td>
<td>191.54</td>
<td>448.24</td>
<td>378.87</td>
<td>381.34</td>
<td>856.61</td>
<td>0.12</td>
<td>1.59</td>
<td>0.99</td>
</tr>
</tbody>
</table>

Fig. 4. Pressure dependence of the elastic constants ($C_{11}, C_{12}$ and $C_{44}$) and the bulk modulus $B$ for UFe₄P₁₂.
expansion coefficient $\alpha$ are given by [45]

$$C_V = 3nK_B \left[ 4D_0 \frac{T}{\theta_D} - \frac{(3\theta_D/T)}{e^{\theta_D/T} - 1} \right]$$

(14)

$$\alpha = \frac{\gamma C_V}{B\theta_D/T}$$

(15)

where $\gamma$ is being the Grüneisen parameter, which is defined as

$$\gamma = - \frac{d\ln(\theta_D(V))}{d\ln V}$$

(16)

Through the quasi-harmonic Debye model, it is possible to calculate the thermodynamic quantities of any temperatures of UFe$_4$P$_{12}$ compound from the calculated $E\!-\!V$ data at $T=0$ and $P=0$.

The average sound velocity $\nu_m$ in the polycrystalline material is given by [46]

$$\nu_m = \left[ \frac{1}{3} \left( \frac{2}{\nu_l^2} + \frac{1}{\nu_t^2} \right) \right]^{1/3}$$

(17)

where $\nu_l$ and $\nu_t$ are longitudinal and transverse speeds of sound obtained using the shear modulus $G$ and the bulk modulus $B$ using Eqs. (18) and (19), respectively [47]

$$\nu_l = \left( \frac{3B + 4G}{3\rho} \right)^{1/2}$$

(18)

$$\nu_t = \left( \frac{G}{\rho} \right)^{1/2}$$

(19)

The symbol $\rho$ is the density obtained from the lattice constants and crystal molecular masses.

Calculations based on LDA approximation for longitudinal and transverse speeds of sound and Debye temperature are documented in Table 4 for UFe$_4$P$_{12}$. It should be noted that there is no experimental or theoretical data in the literature for comparison with our results. Thus, our results can be considered as a prediction of the Debye temperature. Fig. 5 shows the variation of the transverse and longitudinal mean speed, depending on the pressure. It is clear that the longitudinal speed increases linearly with increasing pressure, and form a very steep slope of about 41.15 m/s/GPa, relative to the transverse and average speeds of sound calculated in the order of 13.94 m/s/GPa and 17.50 m/s/GPa respectively.

The specific heat of a material is essential due to the vibrational motion of the ions. However, a small part of heat is due to the motion of free electron, which becomes important at low temperatures, especially in transition metals with electrons in incomplete shells. The specific heat is another important thermal property in the processing operation of casting of heat treatment, since it determines the amount of heat required in the process. The heat capacity of a substance is a measure of how well the substance stores heat. Whenever we supply heat to a material, it will necessarily cause an increase of temperature. This latter parameter provides us essentially an insight into its vibrational properties that are needed for

<table>
<thead>
<tr>
<th>Pressure (GPa)</th>
<th>$\nu_l$ (m/s)</th>
<th>$\nu_t$ (m/s)</th>
<th>$\nu_m$ (m/s)</th>
<th>$\theta_D$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>9284.49</td>
<td>7002.24</td>
<td>7512.815</td>
<td>461.35</td>
</tr>
<tr>
<td>10</td>
<td>9876.74</td>
<td>7244.27</td>
<td>7809.53</td>
<td>575.625</td>
</tr>
<tr>
<td>0</td>
<td>10,368.98</td>
<td>7448.62</td>
<td>8056.71</td>
<td>607.51</td>
</tr>
<tr>
<td>10</td>
<td>10,728.17</td>
<td>7526.18</td>
<td>8169.93</td>
<td>650.96</td>
</tr>
<tr>
<td>30</td>
<td>11,540.46</td>
<td>7817.381</td>
<td>8527.98</td>
<td>710.812</td>
</tr>
<tr>
<td>50</td>
<td>12,222.15</td>
<td>8012.406</td>
<td>8777.717</td>
<td>822.5</td>
</tr>
</tbody>
</table>

Fig. 5. Pressure dependence of the longitudinal, transverse and average sound velocity ($\nu_l$, $\nu_t$, and $\nu_m$, respectively, in m/s) for UFe$_4$P$_{12}$. 

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many applications. A study in this direction is made by Torikachvili for UFe$_4$P$_{12}$ alloy [48].

For UFe$_4$P$_{12}$ material we have investigated the thermal properties in temperature range from 0 to 3000 K, where the quasi-harmonic model remains fully valid. We have also monitored the effect of pressure (in GPa range). In Fig. 6 we present the temperature-dependent behavior of the heat capacity $C_v$ at constant-volume. From this curve, we can distinguish two types of variations: firstly, it is seen that when $T < 500$ K, $C_v$ increases very quickly with temperature. Secondly, beyond this temperature $C_v$ increases slowly with temperature. Beyond 750 K, $C_v$ reaches Dulong–Petit limit and remains constant ($C_v \sim 3R$ for mono atomic solids at higher temperature). However, it can be emphasized that $T^3$ behavior matches Debye model at low temperature.

On the other hand, we have studied the effect of temperature and pressure on the behavior of the thermal expansion $\alpha$ in temperature range 0–500 K at various pressures (−15 to 50 GPa) as shown in Fig. 7. This latter factor presents a rate that increases with increasing temperature. However, the thermal expansion coefficient $\alpha$ shows a sharp decrease with increasing pressure and becomes smaller at higher temperatures and pressures. Beyond 350 K, $\alpha$ presents an almost linear variation with increasing temperature.

Fig. 6. Variation of heat capacity as functions of temperature for UFe$_4$P$_{12}$.

Fig. 7. The variation of thermal expansion coefficient $\alpha$ as function of temperature at various temperatures for UFe$_4$P$_{12}$. 
It is well known that Debye temperature is an important fundamental parameter. It is closely related to many physical properties of materials, such as elastic constants, specific heat and melting temperature. It is the temperature above which the crystal exhibits classical behavior, because the phonon contribution to heat capacity became more important than quantum effect. We have plotted in Fig. 8 the evolution of the latter parameter as function of temperature for different pressures. From Fig. 8, one deduced the value of Debye temperature at zero pressure and zero temperature which is found to be 612 K it is near than calculated by using the elastic constants presented in Table 4 (607.51 K).

Fig. 9 shows the pressure and temperature dependence of the relative volume $V$ for $\text{UFe}_4\text{P}_{12}$. The relative volume $V$ increases with increasing temperature but the rate is more important for temperature above 100 K. On the other side, at a given temperature, the relative volume $V$ decreases.
when the pressure \( P \) increases. The effect of increasing temperature on volume is just the same as decreasing pressure. In Fig. 10, we present the variation of bulk modulus \( B \) with temperature at several pressures. It can be seen that \( B \) is nearly constant from 0 to 100 K and decreases linearly with increasing temperature for \( T = 100 \) K. It indicates thermal softening of the rare earth-filled skutterudites lattice. The compressibility increases with increasing temperature at a given pressure and decreases with pressure at a given temperature. At 300 K and zero pressure, the calculated bulk modulus value for UFe\(_4\)P\(_{12}\) herein studied is 199.227 GPa. We note that at zero pressure, \( B \) is lower than at higher pressures. This essentially implies that the rare earth-filled skutterudites lattice is stiffened with increase in pressure and becomes stiffer at higher pressure. The mechanical stiffened bulk modulus in rare earth-filled skutterudites lattice is attributed to bond compression and bond strengthening due to lattice vibration.

![Fig. 10. The variation of the bulk modulus as function of temperature at different pressures for UFe\(_4\)P\(_{12}\).](image-url)

![Fig. 11. Calculated Gibbs energy of UFe\(_4\)P\(_{12}\) at the pressure is equal to 0 GPa.](image-url)
Fig. 11 represents the Gibbs free energy for UFe$_4$P$_{12}$ calculated in function the temperature. It can be seen from this figure that when the temperature increases, the values of the free energy ($G$) for UFe$_4$P$_{12}$ decreases gradually.

3.4. Electronic properties

The band structure of the uranium filled skutterudite UFe$_4$P$_{12}$ is shown in Fig. 12. Calculated values of band parameters are illustrated in Table 5. Fig. 13 discerns an

![Image](image-url)

*Fig. 12. The calculated electronic band dispersion curves along some high symmetry directions of the Brillouin zone for UFe$_4$P$_{12}$ at 0, 10, 30 and 50 GPa.*
indication of a tendency to form a pseudo-gap that appears above the Fermi level at \( \Gamma \) point, which is a characteristic of Skutterudite, especially when a single phosphorous \( p \)-band crosses the Fermi level. The crossing band is, indeed, pushed down by the repulsion of \( U_f \)-resonance states. \( UFe_4P_{12} \) has been reported as semiconductor, a result attributed to the higher electronegativity of phosphorus contrary to earlier reported insulator characteristic of \( UFe_4P_{12} \). The present calculated band structure depicts a semimetal behavior for \( UFe_4P_{12} \). Furthermore, the calculations of the electronic structure of \( UFe_4P_{12} \) [49] using extended Hückel tight-binding method corroborate this finding. On the other hand, the absence of a mini gap in \( UFe_4P_{12} \) could be attributed to the omission from our calculations of the mean field Hubbard correction, popularly called \( \text{LDA} + U \), which are necessary in this system characterized by strong electronic correlation.

4. Conclusion

In summary, this work contributes to the structural, electronic and elastic properties of \( U \)-based filled skutterudite compound \( UFe_4P_{12} \) by the FP-LMTO method within the DFT. The deduced results are in good agreement with the experimental data found in the literature. We gave a prediction of the Debye temperature \( \theta_D \), shear modulus \( G \), Young’s modulus \( E \), Poisson’s ratio \( \nu \) and the anisotropy parameter \( A \) for \( U \)-based filled skutterudite \( UFe_4P_{12} \). Furthermore, following the quasi-harmonic Debye model, the dependences of the volume, bulk modulus, heat capacities and Debye temperature on temperature and pressure were obtained successfully. Energy bands indicate that \( UFe_4P_{12} \) is a semi-metal with a clear distinction between conduction and valence bands. A very flat band along the symmetry axis \( \Gamma \rightarrow N \) was determined in the range of 0.59 eV at the pressure equal to 0 GPa.

References
