First-Principles Study of ZnIn2Te4 and HgIn2Te4 Defect-Chalcopyrite Semiconductors Under Different Pressures: Electronic, Elastic, And Optical Properties

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First-principles study of ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$ defect-chalcopyrite semiconductors under different pressures: Electronic, elastic, and optical properties

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Abstract

First-principle calculations of electronic, elastic, and optical properties for ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$ defect-chalcopyrite semiconductors have been performed using local density approximation (LDA). Computed energy bandgaps are 1.398 eV and 1.101 eV, respectively, for ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$, which show the indirect bandgaps behavior. Elastic parameters and Debye temperature have also been investigated at 0, 5, 10, 13, and 14 GPa pressures. Calculated results indicate that both semiconductors are covalent in nature at 0 GPa and become ionic afterward. Optical parameters have also been examined under 0, 5, 10, and 13 GPa in the energy span of 0 eV to 15 eV. The calculated values indicate that these semiconductors are mechanically stable up to 13 GPa and become unstable at 14 GPa. The calculated values of all parameters are compared with the available experimental and reported values at 0 GPa. A reasonable agreement has been obtained between them. The values of these parameters at 5, 10, 13, and 14 GPa pressures are reported for the first time.

Keywords: first-principle calculations, defect chalcopyrite, electronic properties, Debye temperature, and optical properties.
1. Introduction

Defect-chalcopyrites (DCs) are special type of semiconductors of $A^{II}B^{III}C^{IV}$ family, which have an ordered vacancy compounds (OCV) structure. They have potential applications in the areas of solar cells, optoelectronics, linear and nonlinear optical devices [1–9]. As a result, much emphasis has been placed on the experimental synthesis and structural characterization of these materials. Experimentally, the Bridgman and chemical vapor transport (CVT) methods have been used to investigate their properties, which are observed by X-ray diffraction and Raman scattering [10–17]. Whereas theoretically, the density functional theory (DFT) has been used by different workers [2–5, 18–20]. Recently, the authors have also used the first-principle calculations to investigate the different linear properties of LiGaS$_2$, LiGaSe$_2$, ZnGeN$_2$ semiconductors [21, 22], and functionalized graphene semiconductors [23]. Various linear [24] and nonlinear optical (NLO) properties [25] of chalcopyrites have also been studied using plasma oscillations theory of solid. So far, no work has been carried out under different pressures. In this paper, we have investigated the effect of pressure on various properties of XIn$_2$Te$_4$ (X= Hg, Zn) defect-chalcopyrites using first-principle calculations. The effect of the pressure on $C_{ij}$, $G$, $B$, $\nu$, $B/G$ ratio, $A$, and $\Theta_D$ parameters have been studied at 0, 5, 10, 13, and 14 GPa. The values of lattice parameter (a, c), anion displacement parameters ($U_x$, $U_y$, and $U_z$), bond lengths ($d_{X-Te}$, $d_{In-Te}$, and $d_{In'-Te}$), energy bandgap ($E_g$), and density of states (DOS) have been calculated at ambient conditions. The optical properties have also been investigated in the energy range of 0 eV to 15 eV at pressures of 0, 5, 10, and 13 GPa. The estimated values of all 23 parameters are reasonably agreed with the known experimental and theoretical data at 0 GPa. The calculated values of these parameters at 5, 10, 13, and 14 GPa pressures are reported for the first time.
2. Computational methods

First-principle calculations within DFT have been done using Cambridge Sequential Total Energy Package (CASTEP) \cite{26} code to estimate linear properties such as electronic, optical, and elastic properties of XIn$_2$Te$_4$ (X = Zn, Hg) under different pressures. The calculations are based on local density approximation (LDA) of the Ceperley and Alder scheme parameterized by Perdew and Zunger to define exchange-correlation functions \cite{27, 28}. The non-conversing pseudo-potentials \cite{29} have been applied with 660 eV cut-off energy for the plane-wave basis set. The reciprocal crystal lattice and Brillouin zone integration have been executed using Monkhorst-pack mesh of 3×3×3 within the Broyden, Fletcher, Goldfarb, and Shanno (BFGS) scheme \cite{30}. Throughout geometry optimization, ultrafine quality for convergence threshold has been applied wherein Hell-Feynman ionic force is 0.01 eV/Å, maximum total energy \(5 \times 10^{-6}\) eV/atom, maximum ion displacement \(5 \times 10^{-4}\) Å, and stress tolerance 0.02 GPa.

3. Results and discussion

3.1. Structural properties

Defect-chalcopyrite semiconductors with formula XIn$_2$Te$_4$ (X = Zn, Hg) have a body-centered tetragonal configuration with space group I-4 (#82). Each unit of XIn$_2$Te$_4$ crystal contains two-X, four-In, and eight-Te atoms along with two vacancies per unit cell. Wyckoff atomic coordinates of XIn$_2$Te$_4$ crystal are X (0, 0, 0), In$^1$ (0, 0, 0.5), In$^2$ (0, 0.5, 0.5) and Te ($U_x$, $U_y$, $U_z$), where $U_x$, $U_y$ and $U_z$ are anion displacement parameters in three axes. The value of lattice parameters has been calculated and listed in Table 1, which are in fair agreement with the available data reported experimentally and theoretically \cite{31, 32}. The tetragonal distortion \(\eta = c/2a\) is 1 for the ideal structure, whereas the calculated values of \(\eta\) are 0.996 and 0.987 for ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$, respectively, which equivalent to 1. This shows the presence of tetragonal distortion. The values
of anion displacement parameters ($U_x$, $U_y$, and $U_z$) and bond lengths ($d_{X-Te}$, $d_{In-Te}$, and $d_{Hg-Te}$) for ZnIn$_2$Te$_4$ and ZnIn$_2$Te$_4$ have been determined and presented in Table 1 along with the known values [8, 19, 33–35]. They agree well with the available reported values in the case of ZnIn$_2$Te$_4$. However, the values of these parameters for HgIn$_2$Te$_4$ are not available for comparison. Further, Table 1 shows that the bond lengths $d_{In-Te}$ and $d_{Hg-Te}$ are larger than $d_{X-Te}$. Figures 1(a) and 1(b) display the approximate band structures of ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$, respectively. This shows that both crystals are direct bandgap semiconductors with a bandgap of 1.398 eV and 1.101 eV along $\Gamma - \Gamma$ direction, respectively for ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$ at ambient conditions. The estimated bandgap $E_g$ values are presented in Table 1, together with known data [7, 8, 19, 31–37]. The estimated values $a$, $c$, $U_x$, $U_y$, $U_z$, and $E_g$ are also in fair concordance with the existing reported and experimental data.

The density of states provides knowledge about a crystal's angular momentum character. The elements Zn, Hg, In, and Te have the electronic configurations [Ar]3d$^{10}$4s$^{2}$, [Xe]4f$^{14}$5d$^{10}$6s$^{2}$, [Kr]4d$^{10}$5s$^{2}$5p$^{1}$ and [Kr]4d$^{10}$5s$^{2}$5p$^{4}$, respectively. In the energy span of -15 eV to 10 eV, the total density of state (TDOS) and partial density of state (PDOS) have been computed and shown in Fig. 2. At 0 GPa pressure, Fig. 2 (a) shows the TDOS and PDOS for the Zn-4s/3p/3d, In-5s/5p, and Te-5s/5p states, which reveals that the valence band is divided into three parts. The first portion is mostly made up of Te-5s, with a small amount of In-5s and In-5p states. The second portion is strongly localized, owing to the presence of Zn-3d in -7.46 eV to -6.44 eV energy region. The valance band, which ranges from -6.09 eV to Fermi energy ($E_F = 0$ eV), is the third and final part. Mainly In-5s/5p and Te-5s/5p states give rise to make the third part. Figure 2 (a) reveals that the
valence band is primarily made up of Zn-4s, Te-5s, and Te-5p states, with In-5s and In-5p making a minor contribution. The major effect of In-5s/5p and Te-5s/5p, with an admixture of Zn-4s/3p/3d, forms the conduction band, which ranges from 1.90 eV to 6.91 eV. The TDOS and PDOS for Hg-6s/5p/5d, In-5s/5p and Te-5s/5p states has been shown in Fig. 2 (b). Figure 2 (b) shows that similar results have also been observed for HgIn$_2$Te$_4$ in the valence and conduction bands.

3.2. Elastic properties

Elastic parameters are essential parameters to convey the mechanical strength of any material. XIn$_2$Te$_4$ crystallizes in the tetragonal structure that comes under the Laue group T11 [4, 5]. Tetragonal Laue group T11 does not have an analytical formula to calculate elastic moduli as it contains off-diagonal shear elastic constant $C_{16}$. Due to this, seven elastic constants are obtained in the optimized structure. However, employing $C_{16}$ equals zero, seven elastic constants of the Laue group T11 can be transformed into six elastic constants of the Laue group T1. Laue group T1 has a well-known formula to calculate the elastic constant from its six elastic stiffness constants $C_{ij}$, i.e., $C_{11}, C_{12}, C_{13}, C_{33}, C_{44}$ and $C_{66}$. Transformation of seven elastic stiffness coefficients of Laue group T11 into six elastic stiffness coefficients of Laue group T1 can be obtained through rotation around the z-axis with the angle given by following relations [4, 5]:

$$\phi_{x,y} = \frac{1}{4} \arctan\left(\frac{4C_{16}}{C_{11} - C_{12} - 2C_{66}}\right)$$

(1)

The above Eq. (1) gives the values of $\phi_x$ and $\phi_y$ within the range $0 < \phi < |\pi/2|$, where $\phi_y = \phi_x + \pi/4$. The value of $\phi_x$ has been calculated using Eq. (1) and found to be 0.87° for ZnIn$_2$Te$_4$ and 2.30° for HgIn$_2$Te$_4$ at 0 GPa. Six independent elastic constants $C_{ij}$ of Laue group T1
have been calculated using relations mentioned in Ref. [38, 39] by employing the LDA estimated seven elastic stiffness coefficients of Laue group T11 and angle $\phi$. The values of these six coefficients, i.e., $C_{11}, C_{12}, C_{13}, C_{33}, C_{44}$ and $C_{66}$ have been calculated at 0, 5, 10, 13, and 14 GPa pressures. For any stable tetragonal Laue group T1 crystal, all six independent elastic stiffness coefficients under pressure must fulfill the Born-Huang criteria as follows [40]:

$$C_{11} - P > 0; \quad C_{44} - P > 0; \quad C_{11} - C_{12} - 2P > 0; \quad (C_{33} - P)(C_{11} + C_{12}) - 2(C_{13} - P)^2 > 0 \quad (2)$$

The estimated values of $C_{ij}$ for $\phi$ at five different pressures are presented in Table 2 for XIn$_2$Te$_4$.

Plots have also been drawn between $C_{ij}$ and pressure, and presented in Figs. 3 (a) and 3 (b), respectively, for ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$. Figure 3 shows that the values of $C_{ij}$ increase with the increasing pressure for both the materials. At 14 GPa, the value of $C_{ij}$ defies the stability criteria mentioned above of Eq. (2) and turns into an unstable form, which indicates that XIn$_2$Te$_4$ is stable up to 13 GPa only. It has also been observed that the values of $C_{11}$ and $C_{33}$ are significantly higher than the values of $C_{12}$, $C_{13}$, $C_{44}$ and $C_{66}$. This shows that the compounds are anisotropic and have more chances of shear deformation in the direction of a- and c- axes than compression deformation.

Further, the value of elastic moduli of ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$, such as shear modulus ($G$), bulk modulus ($B$), Poisson's ratio ($\nu$), $B/G$, and Young's modulus ($E$) have been calculated at 0, 5, 10, 13, and 14 GPa using the relations given in Ref. [41]. The estimated values of these elastic moduli are presented in Table 2. The bulk modulus for ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$ is
35.322 GPa and 33.742 GPa, respectively, based on the extended Cohen formula given in Ref. [3]. The calculated values of bulk modulus $B$ are in good agreement at 0 GPa. Elastic moduli ($B$, $G$ and $E$) versus pressure plots are shown in Fig. 4 (a) and 4 (b) for ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$ respectively, which indicates that $B$, $G$ and $E$ increase with the increase of pressure. Frantsevich et al. [22, 42, 43] have proposed the critical limits of $\nu < 0.33$ and $B/G < 2.67$ for covalent (brittle) materials else it is ionic (ductile). The calculated values of $\nu$ and $B/G$ indicate that both the semiconductors are of covalent behavior at 0 GPa. However, violate the inequalities and show the ionic (ductile) behavior at 5, 10, 13, and 14 GPa pressures. The Zener shear anisotropy factor's value ($A$) has been evaluated using the formula $A = 2C_{66} / (C_{11} - C_{12})$ [44] and presented in Table 2. For an anisotropic material, the value should be $A \neq 1$ otherwise material said to be isotropic material. Our calculated values of $A$ also show the anisotropic character of both compounds.

Debye temperature ($\theta_D$) is a constant that signifies the temperature of the highest form of a crystal's vibration, which is closely related to the specific heat and melting point of the compounds. Using data of $G$ and $B$, Debye temperature values ($\theta_D$) have been estimated based on relations given in Ref. [32, 45]. The calculated values of $\theta_D$ for ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$ have been presented in Table 2, together with the reported data [8]. The calculated value of $\theta_D$ for ZnIn$_2$Te$_4$ is found to be in fair agreement with reported values at 0 GPa [8]. However, the known values of $\theta_D$ for CdIn$_2$Te$_4$ and at other pressure are not available for comparison.

### 3.3. Optical properties

The frequency dependence complex dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ is a prominent part of optical properties, which derives all other optical parameters such as extinction
coefficient $\alpha(\omega)$, reflectivity $R(\omega)$, refractive index $n(\omega)$, and energy loss function $L(\omega)$ using the relations mentioned in the literature [46–49]. The imaginary part $\varepsilon_2(\omega)$ of the complex dielectric function deals with the absorption of the incident photon, and the real part $\varepsilon_1(\omega)$ of the complex dielectric function concerns with the incident photons dispersion. The optical parameters such as the imaginary part $\varepsilon_2(\omega)$ and real part $\varepsilon_1(\omega)$ of complex dielectric function $\varepsilon(\omega)$ for XIn$_2$Te$_4$ have been estimated at 0, 5, 10, and 13 GPa pressures. Curves have also been plotted for $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ parameters in the energy range of 0 – 15 eV and presented in Figs. 5 and 6, respectively, for ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$. The peak values of $\varepsilon_2(\omega)$ and $\varepsilon_1(\omega)$ parameters in Figs. 5 and 6 are marked as 'X,' which shows that in most cases, the peaks move in the direction of the high energy zone (blue-shift) with a change of pressure from 0 GPa to 5 GPa, 5 GPa to 10 GPa, and 10 GPa to 13 GPa. Further, the static dielectric constant $\varepsilon(0)$ has been calculated and presented in the last row of Table 2. A fair agreement has been found between them at 0 GPa [50]; however, they await experimental verification at other pressures.

Figs. 5 (a), 5 (b), and Fig. 5
Figs. 6 (a), 6 (b), and Fig. 6

4. Conclusions

The first-principle study is executed effectively to calculate the electronic, elastic, and optical properties for defect-chalcopyrite ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$ semiconductors at 0, 5, 10, 13, and 14 GPa pressures. The estimated values of electronic parameters such as lattice parameter (a and c), energy bandgap ($E_g$), anion displacement parameter ($U_x$, $U_y$, and $U_z$), and bond lengths ($d_{X-Te}$, $d_{In^1-Te}$, and $d_{In^2-Te}$) are presented in Table 1, which agree well with available reported and experimental values. The band structure shows that both compounds are indirect semiconductors
with an energy gap of 1.398 eV and 1.101 eV, respectively, for ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$. The TDOS and PDOS plots of ZnIn$_2$Te$_4$/HgIn$_2$Te$_4$ demonstrate that Zn/Hg has a marginal effect around the Fermi level. However, the Te-5s/5p and In-5s/5p states dominate in the forming of valance and conduction bands. The value of $C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, G, B, E, A, \nu, B/G$ and $\theta_p$ have been estimated at 0, 5, 10, 13, and 14 GPa pressures and summarized in Table 2. The values of $C_6$ indicate that ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$ are stable up to 13 GPa and later becomes unstable. The calculated values of $\nu$ and $B/G$ for ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$ are smaller than the critical limits of 0.33 and 2.67 at 0 GPa, which demonstrate the covalent behavior. Moreover, the estimated data of $\nu$ and $B/G$ do not satisfy the criterion of critical limits at 5, 10, and 13 GPa, and hence show the presence of ionic behavior. The estimated values of static dielectric constant $\varepsilon(0)$ are listed in Table 2 at 0, 5, 10, and 13 GPa pressures, which indicates that the values of $\varepsilon(0)$ increase with the increasing pressure. The calculated static dielectric constant data under three different pressures of 5, 10, and 13 GPa are not available for comparison, as well as 12 elastic parameters and Debye temperature under four different pressures of 5, 10, 13, and 14 GPa are stated for the first time which await for experimental verification. The predicted values are generally in strong alignment with experimental and previously reported values, demonstrating the importance of this computational work. The values of these parameters are critical for future technological applications, such as selecting substrate materials and designing integrated circuits (ICs) for electro-optic systems. The predictive description of the computational methodology introduced in the present work is of immense significance and will mentor the forthcoming studies of these properties of new defect-chalcopyrite materials belong to the A$^{II}$B$_2^{III}$C$_4^{VI}$ family.
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**Conflict of interest** The authors declare no conflicts of interest.

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Table 1. Optimized values of lattice parameters (a=b and c), unit cell volume ($V_0$), internal parameters ($U_x$, $U_y$ and $U_z$), bond lengths ($d_{X-Te}$, $d_{In-Te}$ and $d_{Hg-Te}$), and energy bandgap ($E_g$) for ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$ defect-chalcopyrite semiconductors.

| Compounds         | a (Å) | c (Å) | $V_0$(Å$^3$) | $U_x$ | $U_y$ | $U_z$ | $d_{X-Te}$(Å) | $d_{In-Te}$(Å) | $d_{Hg-Te}$(Å) | $E_g$(eV) |
|-------------------|-------|-------|--------------|-------|-------|-------|---------------|----------------|----------------|----------|
| ZnIn$_2$Te$_4$    |       |       |              |       |       |       |               |                |                |          |
| This work         | 6.045 | 12.044| 434.517      | 0.270 | 0.218 | 0.137 | 2.655         | 2.734          | 2.726          | 1.398     |
| Expt.             | 6.11$^b$, 6.132$^b$ | 12.22, 12.29$^b$ | 0.26$^b$ | 0.24$^b$ | 0.13$^b$ | 1.87–1.90$^c$ |
| Rep.              | 6.122$^c$, 6.494$^c$, 6.12$^d$, 6.11$^e$ | 12.24, 12.88$^c$, 12.24, 12.22$^d$ | 0.248$^c$, 0.261$^c$, 0.25$^d$, 0.269$^d$ | 0.250$^c$, 0.221$^c$, 0.25$^d$, 0.208$^d$ | 0.1256$^c$, 0.130$^e$, 0.125$^e$, 134$^e$ | 1.90$^f$, 1.4$^f$ |
| HgIn$_2$Te$_4$    |       |       |              |       |       |       |               |                |                |          |
| This work         | 6.125 | 12.084| 446.833      | 0.277 | 0.225 | 0.141 | 2.757         | 2.736          | 2.726          | 1.101     |
| Expt.             | 6.17$^b$ | 12.3$^b$ |              |       |       |       |               |                |                |          |
| Rep.              | 6.186$^d$ | 12.3$^d$ |              |       |       |       |               |                |                | 1.37$^d$ |

$^a$Reference [31]. $^b$Reference [33]. $^c$Reference [36]. $^d$Reference [32]. $^e$Reference [19]. $^f$Reference [34]. $^g$Reference [8]. $^h$Reference [35]. $^i$Reference [7]. $^j$Reference [37]

Table 2. Calculated values of elastic constants $C_{ij}$ in GPa, bulk modulus $B$ in GPa, Shear modulus $G$ in GPa, Young’s modulus $E$ in GPa, Poisson’s ratio $\nu$, $B/G$ ratio, Zener anisotropy factor $A$ and Debye temperature $\theta_D$ in °K under different pressure for ZnIn$_2$Te$_4$ and HgIn$_2$Te$_4$.

| Elastic parameters | ZnIn$_2$Te$_4$ | HgIn$_2$Te$_4$ |
|--------------------|----------------|----------------|
|                    | At 0 GPa       | This work at   | At 0 GPa       | This work at   |
|                    | This work      | 5 GPa          | 10 GPa         | 13 GPa         | 14 GPa         | 5 GPa          | 10 GPa         | 13 GPa         | 14 GPa         |
| $C_{11}$           | 71.59          | 101.15         | 129.06         | 125.87         | 138.56         | 61.27          | 90.39          | 116.08         | 127.40         | 125.80         |
| $C_{33}$           | 52.53          | 81.88          | 95.77          | 107.90         | 109.51         | 53.19          | 79.56          | 101.32         | 109.75         | 115.63         |
| $C_{44}$           | 28.91          | 36.00          | 39.14          | 30.35          | 22.46          | 24.32          | 35.71          | 38.78          | 20.53          | 26.08          |
| $C_{66}$           | 13.74          | 20.63          | 19.79          | 38.35          | 24.08          | 13.06          | 27.62          | 32.00          | 26.89          | 30.44          |
| $C_{12}$           | 23.60          | 49.05          | 65.69          | 94.78          | 88.69          | 19.90          | 58.59          | 85.76          | 87.94          | 95.02          |
| $C_{13}$           | 29.93          | 52.34          | 74.22          | 85.67          | 90.80          | 27.62          | 56.01          | 79.17          | 88.92          | 95.01          |
| $B$                | 39.27          | 35.322$^d$     | 64.44          | 85.21          | 97.27          | 101.28         | 35.61          | 33.742$^d$     | 65.71          | 89.64          | 98.33          | 103.34         |
| $G$                | 20.79          | 26.40          | 27.15          | 24.60          | 21.24          | 18.48          | 24.18          | 25.73          | 19.89          | 20.88         |
| $E$                | 53.02          | 69.69          | 73.64          | 68.07          | 59.57          | 47.26          | 64.61          | 70.45          | 55.91          | 58.69          |
| $\nu$              | 0.27           | 0.32           | 0.36           | 0.38           | 0.40           | 0.28           | 0.34           | 0.37           | 0.41           | 0.41          |
| $B/G$              | 1.89           | 2.44           | 3.14           | 3.95           | 4.77           | 1.93           | 2.72           | 3.48           | 4.94           | 4.95          |
| $A$                | 0.50           | 0.67           | 0.55           | 1.93           | 0.85           | 0.56           | 1.39           | 1.60           | 1.14           | 1.66          |
| $\theta_D$         | 195.376        | 175$^e$        | 221.411        | 225.617        | 215.569        | 200.824        | 172.736        | 199.037        | 206.240        | 182.256        | 186.729       |
| $\varepsilon(0)$   | 11.885         | 7.1±0.3$^a$    | 13.348         | 14.566         | 15.730         | 10.407         | 8.55$^a$       | 11.860         | 13.076         | 13.756        |

$^a$Reference [50]. $^b$Experimental value, $^c$Value calculated based upon extended Cohen formula given in Ref. [3]
Fig. 1. Electronic band structure of (a) ZnIn$_2$Te$_4$ (1.398 eV) and (b) HgIn$_2$Te$_4$ (1.101 eV).
Fig. 2. DOS for (a) ZnIn$_2$Te$_4$ and (b) HgIn$_2$Te$_4$. 
Fig. 3. Elastic constants vs pressure curve for (a) $\text{ZnIn}_2\text{Te}_4$ and (b) $\text{HgIn}_2\text{Te}_4$. 
Fig. 4. (a) Elastic moduli vs pressure curve for (a) ZnIn$_2$Te$_4$ and (b) HgIn$_2$Te$_4$. 
Fig. 5. Optical properties of ZnIn$_2$Te$_4$: (a) real part dielectric function and (b) imaginary part of the dielectric function.
Fig. 6. Optical properties of HgIn$_2$Te$_4$: (a) real part dielectric function and (b) imaginary part of the dielectric function.