PAPER

Ab initio investigations of structural, elastic, electronic and optical properties of the fluoroperovskite TIXF₃ (X=Ca, Cd, Hg, and Mg) compounds

Sajid Khan ¹, Shams U Zaman ¹, Rashid Ahmad ¹✉, Nasir Mehmood ¹, Muhammad Arif ² and H J Kim³

¹ Department of Physics, Kohat University of Science and Technology, Kohat 26000, Khyber Pakhtunkhwa, Pakistan
² Faculty of Materials Science and Engineering, Kunming University of Science and Technology, Kunming, 650093, People’s Republic of China
³ Department of Physics, Kyungpook National University, Daegu, 41566, Republic of Korea

E-mail: rashidahmad@kust.edu.pk

Keywords: density functional theory, Fluoroperovskite, electronic properties, elastic properties, optical properties

Abstract

Ab initio calculations of Tl-based fluoroperovskite compounds TIXF₃ (X = Ca, Cd, Hg, and Mg) are carried out in the framework of Density Functional Theory (DFT). We have investigated their structural, elastic, electronic and optical properties using the full-potential linearized augmented plane wave (FP-LAPW) method. The exchange-correlation potential is examined using the generalized gradient approximation with additional Hubbard-U term for indulging on-site Coulomb interaction (GGA+U). These compounds have been found to be mechanically stable. The elastic properties such as elastic constants, bulk modulus, anisotropy factor, Poisson’s ratio, and Pugh’s ratio are obtained. The calculations of electronic band structure show that the TlCaF₃ and TlMgF₃ are direct while TlCdF₃ and TlHgF₃ are indirect band gap materials. The contribution of the different bands was analyzed from the total and partial density of state curves. Calculations of the optical spectra such as the real and imaginary parts of the dielectric function, optical reflectivity, absorption coefficient, optical conductivity, refractive index and extinction coefficients are performed for the energy range of 0 to 30 eV.

1. Introduction

Compounds having general chemical composition ABF₃ are well known as fluoroperovskites. In ABF₃, A and B represent cations while F (Fluorine) is an anion. These compounds form an interesting class of materials with mechanically stable crystal structure while showing good electronic behavior having band gap energy ranging from semiconductors to insulators. These compounds have received much attention in recent years due to their technological importance as a lens material in optical lithography, scintillation materials, radiation dosimeters and in semiconductor industry [1–3]. Owing to such broad applications, these compounds are widely examined experimentally and computationally by different authors e.g. see in [4].

Fluoroperovskites are generally characterized by their large energy band gap [5–7]. The wide energy gap of these compounds makes them technologically important. KMgF₃ and BaLiF₃ are used as vacuum-ultra-violet materials for lenses in optical lithography steppers [8, 9]. KMgF₃ is also promising as a scintillation material [2] and radiation dosimeter [10] when doped with lanthanide ions Ce and Er. Theoretical study on Ag-based fluoroperovskites, AgMgF₃ and AgZnF₃, was reported by Murtaza et al [11]. They predicted wide absorption energy range of reported materials make them suitable for different device applications. The optoelectronic properties of Sn–based fluoroperovskites were studied in [12]. These compounds were found to be electronically insulators and were predicted to have Auger–Free luminescence (AFL). Structural, magnetic and optoelectronic behavior of TlMnX₃ (X = Cl, and F) were reported by F Hamioud et al in [13] and optics technology applications were predicted based on optical spectra. A simulation study on TlCdF₃ revealed its
insulating nature, having transparency for a wide range of energies and therefore suggesting it suitable for optical applications [14]. Despite interest in the investigation of fluoroperovskite compounds for various applications, to the best of our knowledge, there is a lack of literature on the study of Tl-based fluoroperovskites. A recent trend in the development of thallium based compounds in the field of radiation detection is observed and various studies have been reported [15, 16]. The presence of thallium atom in the chemical composition of these compounds increases the effective atomic number that contributes towards better detection efficiency [17]. Moreover, the simple cubic structure of the compounds makes them technologically promising candidate in the applications where single growth is required.

In this study, we aim to give a detailed description of the structural, elastic, electronic and optical properties of TlXF3 (X = Ca, Cd, Hg and Mg) compounds using the GGA + U method. This approach in DFT was proposed in the 90s to treat the electronic correlation with the Hubbard-like model [18]. Since then, it has been widely used to investigate the properties of various materials [19–21] including halide perovskites [22].

This paper is organized in 4 sections. Section 2 is devoted to the method of calculation, in section 3, results and discussions are presented and finally, section 4 is devoted to the conclusions of the study.

2. Methodology

The ternary fluorоперовскит TlXF3 (X = Ca, Cd, Hg, and Mg) compounds have cubic perovskite type structure with space group Pm-3m (#221). The unit cell comprises of one molecule with Tl and X positioned at (0, 0, 0) and (0.5, 0.5, 0.5), respectively, and the three F atoms are at (0.5, 0, 0.5), (0, 0.5, 0.5) and (0.5, 0.5, 0) sites of the Wyckoff coordinates as shown in figure 1.

Simulation study for the investigation of structural, elastic, electronic and optical properties is carried out by applying the general framework of density functional theory (DFT). The full potential linearly augmented plane wave (FP-LAPW) technique [23] is implemented by employing WIEN2K code [24]. The effect of on-site Coulomb interactions is considered and calculations are performed in generalized gradient approximation with additional Hubbard-U term for indulging on-site Coulomb interaction (GGA + U) [25]. Structural parameters are investigated by fitting the energy versus volume curve using Murnaghan’s equation of state [26]. For this study, the value of RMT is chosen in such a manner that there is no charge leakage from the core and the total energy is ensured. RMT values of 2.5, 2.01, 2.12, 2.18 and 1.85 are used for Tl, Ca, Cd, Hg and Mg while RMT values for F in TlCaF3, TlCdF3, TlHgF3 and TlMgF3 are 2.01, 1.88, 1.94 and 1.85 respectively. The wave function within muffin tin spheres are expanded in spherical harmonics up to lmax = 10, while K points are taken to be 1000 and Γmax is 12. The difference of energy between the core and valence band is taken as 6 Ry.
3. Results and discussion

3.1. Structural and elastic properties

All Tl-based fluoroperovskite compounds studied in this work have ideal cubic structure as shown in figure 1. The variation of total energies with respect to volume is shown in figure 2. The equilibrium lattice constants are obtained by fitting the Birch-Murnaghan equation of state [26]. These values are listed in table 1. In case of TlCdF₃, our calculated lattice constant (4.49 Å) is in reasonable agreement with the value (4.395 Å) found experimentally in [27]. Due to unavailability of the experimental results concerning the equilibrium lattice constants of the rest of studied compounds, we support our calculated results on the basis of known lattice

![Figure 2: Dependence of total energy of Tl-based cubic perovskites TlXF₃ (X = Ca, Cd, Mg, Hg).](image)

| Parameters | TiCaF₃ | TiCdF₃ | TiHgF₃ | TiMgF₃ |
|------------|--------|--------|--------|--------|
| a₀        | 4.94   | 4.49   | 4.61   | 4.15   |
| C₁₁       | 127.21 | 106.62 | 83.23  | 136.75 |
| C₁₂       | 32.78  | 46.89  | 18.53  | 53.81  |
| C₄₄       | 14.28  | 18.09  | 17.90  | 51.22  |
| A         | 0.30   | 0.60   | 0.55   | 1.23   |
| B         | 64.25  | 66.80  | 40.10  | 81.45  |
| G         | 23.63  | 22.13  | 22.74  | 47.07  |
| E         | 63.16  | 59.81  | 57.37  | 118.40 |
| ν         | 0.47   | 0.50   | 0.36   | 0.35   |
| B/G       | 2.71   | 3.01   | 1.76   | 1.73   |
constant of TlMnF$_3$ [13]. As Tl and F atoms in the unit cell are the same in our studied compound and those reported in the [13], the lattice constant should increase as the size of the third atom increases. The ionic radius of Mn$^{2+}$ ion is smaller than Mg$^{2+}$, Cd$^{2+}$, Ca$^{2+}$, and Hg$^{2+}$, that’s why the ionic radii of all our compound have a larger lattice constant values compared to the lattice constant of TlMnF$_3$, which is reported to be 4.123 Å.

Crystal response to applied forces is determined by the elastic constants which provide important information about the mechanical properties of solid materials. For cubic symmetry crystals, three independent elastic constants $C_{11}$, $C_{12}$ and $C_{44}$ are used to determine the mechanical properties such as the rigidity and stability of material under study. The calculated values of elastic constants $C_{ij}$ are presented in table 1. For isotropic materials, this factor is equal to 1 and deviation of values from 1 represents a measure of anisotropy possessed by the material. The calculated values of anisotropy factors are listed in table 1.

The values for TlCaF$_3$, TlCdF$_3$ and TlHgF$_3$ are 0.032, 0.605 and 0.553, respectively while that of TlMgF$_3$ is 1.23. The material is ductile if the $\nu$ is greater than 0.26 otherwise it is brittle. The values listed in table 1 again confirmed that all compounds show ductile nature. The elastic anisotropy factor $A$ for all studied compounds is presented in table 1. For isotropic materials, this factor is equal to 1 and deviation of values from 1 represents a measure of anisotropy possessed by the material. The calculated values of anisotropy factors are listed in table 1. The values for TlCaF$_3$, TlCdF$_3$ and TlHgF$_3$ are 0.032, 0.605 and 0.553, respectively while that of TlMgF$_3$ is 1.23. These results clearly reveal that all compounds are anisotropic. The ductile and anisotropic behavior is in agreement with the similar Tl-based fluoroperovskite compound TlMnF$_3$ [13].

The bulk modulus $B$ can be calculated from elastic constants using the relation

$$B = \frac{C_{11} + 2C_{12}}{3}$$

All the elastic constants are positive and satisfy the criteria $C_{11} > 0; C_{44} > 0; (C_{11} - C_{12}) > 0; (C_{11} + 2C_{12}) > 0; C_{12} < B < C_{11}$ for mechanical stability [29]. Table 1 presents the results of anisotropy factor $A$, Young’s modulus $E$, Poisson’s ratio $\nu$ and Pugh’s index ratio $B/G$ by using the following relations [30].

$$A = \frac{2C_{44}}{C_{11} - C_{12}}$$

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

$$\nu = \frac{3B - 2G}{2(2B + G)}$$

$$G = \frac{G_r + G_b}{2}$$

$$G_r = \frac{C_{11} - C_{12} + 3C_{44}}{5}$$

$$G_b = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})}$$

The classification of a material as a ductile or brittle can be made on the basis of the $B/G$ ratio [31]. If this ratio is smaller than 1.75, the material shows brittle nature otherwise it shows ductile character. On the basis of Pugh’s criteria, all the compounds show ductile nature. Ductility or brittleness of compounds can also be inferred from the poison’s ratio $\nu$ [32].

The material is ductile if the $\nu$ is greater than 0.26 otherwise it is brittle. The values listed in table 1 again confirmed that all compounds show ductile behavior. The elastic anisotropy factor $A$ for all studied compounds is presented in table 1. For isotropic materials, this factor is equal to 1 and deviation of values from 1 represents a measure of anisotropy possessed by the material. The calculated values of anisotropy factors are listed in table 1. The values for TlCaF$_3$, TlCdF$_3$ and TlHgF$_3$ are 0.032, 0.605 and 0.553, respectively while that of TlMgF$_3$ is 1.23. These results clearly reveal that all compounds are anisotropic. The ductile and anisotropic behavior is in agreement with the similar Tl-based fluoroperovskite compound TlMnF$_3$ [13].

### 3.2. Electronic properties

In this section, we are reporting the energy band structure and density of states of compounds under study. The calculated band structure for TlX$_2F_3$ (X = Ca, Cd, Hg, and Mg) along with symmetry directions in the first Brillion zone at equilibrium geometry are given in figure 3. The zero energy is set to coincide with the top of the valence band.

The calculated band gap values for all compounds are found to be 4.39, 3.46, 3.05 and 4.40 for TlCaF$_3$, TlCdF$_3$, TlHgF$_3$, TlMgF$_3$, respectively as listed in table 2 using GGA + U. Figure 3(a) shows that both conduction band minima and valence band maxima of TlCaF$_3$ are located at same X symmetry point in Brillion Zone, exhibiting the direct band gap nature. The band structure of TlCdF$_3$ is presented in figure 3(b) with conduction band minima occurring at $\Gamma$ symmetry point while valence band maxima lying at M symmetry point showing indirect band nature. The indirect band nature is consistent with previous study on TlCdF$_3$ [14]. The band gap nature of TlHgF$_3$ is also indirect as shown in figure 3(c) where conduction band minima and valence minima occur at different points.
Figure 3. The calculated band structure of TlXF$_3$ ($X = \text{Ca, Cd, Hg, and Mg}$) in high symmetry directions.

Table 2. Calculated energy band gap $E_g$ (eV) at high symmetry points for TlXF$_3$ ($X = \text{Ca, Cd, Hg, and Mg}$) by using GGA + U.

| Compound   | $E_{\Gamma}^{\text{M-M}}$ | $E_{\Gamma}^{X-X}$ | $E_{\Gamma}^{\Gamma-I}$ | $E_{\Gamma}^{I-I}$ | $E_{\Gamma}^{\Gamma-X}$ |
|------------|--------------------------|--------------------|------------------------|-------------------|------------------------|
| TlCaF$_3$  | 5.24                     | 4.39               | 6.94                   | 5.82              | 6.69                   |
| TlCdF$_3$  | 5.21                     | 3.67               | 3.46                   | 6.19              | 3.23                   |
| TlHgF$_3$  | 4.19                     | 3.68               | 3.05                   | 5.21              | 2.44                   |
| TlMgF$_3$  | 5.69                     | 4.40               | 8.86                   | 8.08              | 5.89                   |
band maxima are located at \( \Gamma \) and M symmetry points respectively. In the case of TlMgF\(_3\), as shown in figure 3(d), both conduction band minima and valence band maxima are lying at X symmetry point showing direct bandgap nature.

A deeper insight into the electronic structure is obtained by studying the total and partial density of states (TDOS and PDOS) as presented in figure 4. The density of states plot for TlCaF\(_3\) shows that the valence band is dominated by F-p state having a minor contribution from Tl-s state. In conduction band, the major contribution is from Tl-s state. In the case of TlCdF\(_3\), the valence band is populated by F-p and Cd-d states. The conduction band is dominated by states contributed by Cd. Similar to TlCdF\(_3\), the valence band of TlHgF\(_3\) has a major contribution from F-p and Hg-d states. The conduction band states are consisting of F-p and Hg-d states. The DOS plot of TlMgF\(_3\) shows that valence band is mainly populated by F-p while significant contribution is also coming from Tl-s state. In the conduction band, Tl-s state is having a major contribution.

3.3. Optical properties

All the calculations for optical properties are carried out using the GGA + U approach. The photon energy range for optical response is taken as 0–30 eV. The optical properties of the compound can be described by the complex dielectric function represented by the Ehrenreich and Cohen’s equation \([33]\):

\[
\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)
\]

The real part of the dielectric function is calculated by using the equation

\[
\varepsilon_1(\omega) = 1 + \frac{2}{\pi} \int_0^\infty \omega' \frac{\varepsilon'_2(\omega')}{\omega'^2 - \omega^2} d\omega'
\]

The imaginary part can be extracted from the real part by using the Kramers-Kroning relation

\[
\varepsilon_2(\omega) = \frac{8}{2\pi\omega^2} \sum_{m \neq 0} |\mathbf{p}_{m\omega}(k)|^2 \frac{dS_k}{\mathbf{\nabla}\omega_{m\omega}(k)}.
\]

The real part shows the dispersive behavior from the material’s surface and imaginary part shows the absorption of light for the material \([34]\). The absorption of light found from imaginary part represents the optical transitions between the energy bands \([35]\). The real and imaginary part of dielectric functions are used for the calculation of other optical parameters such as refractive index, extinction coefficient, the absorption coefficient, optical conductivity and reflectivity \([36, 37]\). Figure 5 shows that the compounds are optically more...
active in the energy between 3 eV to 8 eV where we see two sharp peaks at about 3 eV and 8 eV. The optical activity in the high energy regime remains below 3 eV.

3.3.1. Refractive index and extinction coefficient

The refractive index and extinction coefficient can be calculated using the following equations [38]

\[
n(\omega) = \left[ \frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}}{2} + \frac{\varepsilon_1(\omega)}{2} \right]^{1/2}
\]

\[
k(\omega) = \left[ \frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}}{2} - \frac{\varepsilon_1(\omega)}{2} \right]^{1/2}
\]

In the figure 6, we see that the refractive index is behaving quite similar to the dielectric function of the materials. It has peaks at about 3 and 8 eV. Two smaller peaks are also observed at about 26 eV for the compound TlCaF$_3$. The refractive index and the extinction coefficients show almost similar behavior but extinction coefficient is smaller than the respective refractive index lower in every energy region. These peaks are due to intraband transitions between valance and conduction bands.

3.3.2. Absorption coefficient

The absorption coefficient contains a contribution from both real and imaginary parts of the dielectric function

\[
I(\omega) = \sqrt{\omega} \left| \sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega) \right|^{1/2}
\]

The absorption coefficient for a material depicts the light absorbed per unit length by an optical system [39]. The absorption is the result of interaction between electrons and photons together with interband and intraband transitions. We see that in figure 7, absorption coefficient has several peaks for all the compounds. TlMgF$_3$ seems to be more active than all other three compounds however TlCaF$_3$ has a maximum peak at about 26 eV.
3.3.3. Reflectivity
The reflectivity is calculated from the imaginary part of the dielectric function

\[ \sigma(w) = \frac{2W_{c}h\omega}{E_{c}} \]  \hspace{1cm} (14)
Figure 8 shows that there is more optical reflectivity in the low energy region than in the high energy. We find several peaks with the highest peak at around 7 eV for the compound TlMgF₃.

3.3.4. Optical conductivity
The optical conductivity is calculated from the following equation

\[ R(\omega) = \frac{n + ik - 1}{n + ik + 1} \] (15)
In the figure 9, we see that the compound TlCaF$_3$ is more active in the high energy region as compared to all other compounds which are active in the low energy region.

4. Conclusions

Structural, elastic, electronic and optical properties of TIXF$_3$ (X = Ca, Cd, Hg, and Mg) are reported in the present work using GGA + U approximations. The equilibrium lattice constants are found to be in the range of 4.15–4.94 Å. The elastic properties such as elastic constants, bulk modulus, anisotropy factor, Poisson’s ratio, and Pugh’s ratio are predicted. The B/G ratio shows that all the studied compounds are ductile in nature. The ductile nature is also confirmed from the obtained values of the Poisson ratio. Our calculations show that TlCaF$_3$ and TlMgF$_3$ have direct bandgap behavior at X-symmetry point, while TlCdF$_3$ and TlHgF$_3$ exhibit indirect band nature. The calculated results are compared and found consistent with available experimental and theoretical data. On the basis of simple cubic structure, large effective atomic number due to the presence of thallium and nature. The calculated results are compared and found consistent with available experimental and theoretical data. On the basis of simple cubic structure, large effective atomic number due to the presence of thallium and nature. The calculated results are compared and found consistent with available experimental and theoretical data.

ORCID iDs

Rashid Ahmad © https://orcid.org/0000-0001-5945-0549

References

[1] Nishimatsu T et al 2002 Band structures of perovskite-like fluorides for vacuum-ultraviolet-transparent lens materials Jpn. J. Appl. Phys. 41 10–3
[2] Hoshina T 2005 5d-level energies of Ce$^{3+}$ and the crystalline environment. I. Fluoride compounds J. Phys. Soc. Japan 48 1261–8
[3] Dotzler C, Williams G V M and Edgar A 2007 RbCdF$_2$: Mn$^{2+}$: a potential ultraviolet dosimeter material Appl. Phys. Lett. 91 36–9
[4] Korbé S, Marques M A L and Botti S 2016 Stability and electronic properties of new inorganic perovskites from high-throughput ab initio calculations J. Mater. Chem. C 4 3157–67
[5] Clouit N, Korba S A, Slimani M, Meradji H, Ghemid S and Khenata R 2013 First-principles study of the structural, electronic and thermal properties of CaLiF$_3$ Phys. Scr. 88 035702
[6] Schedik T, Khenna R, Meradji H, Bouhemsadou A, Bin-Orman S and Rached D 2012 Elastic, electronic and thermodynamic properties of fluoro-perovskite KZnF$_3$ via first-principles calculations Appl. Phys. A 106 645–53
[7] Harmel M et al 2015 Ab initio study of the mechanical, thermal and optoelectronic properties of the cubic CsCdF$_3$, Acta Phys. Pol. A 128 34–42
[8] Vaitheeswaran G et al 2007 High-pressure structural, elastic, and electronic properties of the scintillator host material KMg F$_3$, Phys. Rev. B 76 1–6
[9] Korba S A, Meradji H, Ghemid S and Bouhafs B 2009 First principles calculations of structural, electronic and optical properties of BaLiF$_3$, Comput. Mater. Sci. 44 1265–71
[10] Furetta C, Santopietro F, Sanjipoli C and Kitis G 2001 Thermoluminescent (TL) properties of the perovskite KMgF$_3$ activated by Ce and Er impurities. Appl. Radiat. Isot. 55 533–42
[11] Murtaza G et al 2011 First principle study of cubic perovskites: Ag$\text{TiF}_3$ (T = Mg, Zn) Phys. B Condens. Matter 406 4584–9
[12] Khan I, Shehzad N, Ahmad I, Ali N and Jalali-Asadabadi S 2017 First-principle studies of the optoelectronic properties of ASnF$_3$, (A = Na, K, Rb and Cs) Int. J. Mod. Phys. B 31 1750148
[13] Hamidouf F, Alghamdi G S, Al-Omari S and Mubarak A A 2016 Ab initio investigation of the structural, electronic, magnetic and optical properties of the perovskite TiMnX$_3$ (X = F, Cl) compounds Int. J. Mod. Phys. B 30 1650031
[14] Cheryet A, Lagoun B, Halit M, Zaabar M, Abdelhamim C and Hamza L 2019 First-principles study of structural, electronic, optical and elastic properties of cadmium based Fluoro-Perovskite MCdF$_3$ (M = Rb, Th) Solid State Phenom. 297 175–86
[15] Kim H J, Rooh G, Park H and Kim S 2015 Luminescence and scintillation properties of the new Ce-doped Tl$_3$LiGdCl$_6$ single crystals J. Lumin. 164 86–9
[16] Khan A, Rooh G, Kim H J and Kim S 2018 Ce$^{3+}$-activated Tl$_2$GdCl$_6$: novel halide scintillator for x-ray and γ-ray detection J. Alloys Compd. 741 878–82
[17] Rodnyi P A 1997 Physical Processes in Inorganic Scintillators. (New York: CRC Press)
[18] Liechtenstein A I, Anisimov V I and Zaanen J 1995 Density-functional theory and strong interactions: orbital ordering in Mott-Hubbard insulators Phys. Rev. B 52 R3467–70
[19] German E, Faccio R and Mombru A W 2017 A DFT + U study on structural, electronic, vibrational and thermodynamic properties of TiO$_2$: polymorphs and hydrogen titane: tuning the Hubbard ’U-term’ J. Phys. Commun. 1 035006
[20] Crespo R G, Corà F, Sokol A, de Leeuw N H and Catlow C R A 2006 Electronic structure and magnetic coupling in FeSbO$_3$: a DFT study using hybrid functionals and methods Phys. Rev. B 73 035116
[21] Cinquini F, Giordano I, Puchonni G, Ferrari A M, Pisanu C and Roetti C 2006 Electronic structure of NiO / Ag (100) thin films from DFT + U and hybrid functional DFT approaches Phys. Rev. B 74 165403
[22] Welch E, Scolfaro L and Zakhidov A 2016 Density functional theory + U modeling of polarons in organohalide lead perovskites AIP Adv. 6 125037
[23] Singh D J and Lars N 2006 Plane Waves, Pseudopotentials and LAPW Method. (New York: Springer)
[24] Bhatla P, Schwarz K, Madsen G K H, Kvasnicka D and Luizi T 2001 An Augmented Plane Wave Plus Local Orbitals Program for Calculating Crystal Properties ed K Schwarz (Austria: Techn. Universität Wien) (http://citeulike.org/user/rcolley/article/6205108)
[25] Perdew J P, Burke K and Ernzerhof M 1996 Generalized gradient approximation made simple Phys. Rev. Lett. 77 3865–8
[26] Murnaghan F D 1944 The compressibility of media under extreme pressure Proc. Natl Acad. Sci. USA 30 244–7
[27] Rousseau M, Gesland J Y, Julliard J, Nouet J, Zarembowitch J and Zarembowitch A 1975 Crystallographic, elastic, and Raman scattering investigations of structural phase transitions in RbCdF₃ and TlCdF₃ Phys. Rev. B 12 1579–90
[28] Berger J, Hauret G and Rousseau M 1978 Brillouin scattering investigation of the structural phase transition of TlCdF₃ and RbCaF₃ Solid State Commun. 25 569–71
[29] Grimvall G 1999 Thermophysical Properties of Materials. (Amsterdam: Elsevier)
[30] Hill R 1952 The elastic behaviour of a crystalline aggregate Proc. Phys. Soc. Sect. A 65 349–54
[31] Pugh S F 1954 XCI. Relations between the elastic moduli and the plastic properties of polycrystalline pure metals London, Edinburgh, Dublin Philos. Mag. J. Sci. 45 823–43
[32] Frantsevich and I. N. 1982 Elastic Constants and Elastic Moduli of Metals and Insulators. (Kiyv: Naukova Dumka)
[33] Ambrosch-Draxl C and Sofo J O 2006 Linear optical properties of solids within the full-potential linearized augmented plane-wave method Comput. Phys. Commun. 175 1–14
[34] Makhdoom M et al 2019 First-principles description of the different phases in the Li₃NH compound: electronic structure and optical properties J. Korean Phys. Soc. 74 1140–5
[35] Irfan M et al 2019 Electronic structure and optical properties of TaNO: an ab initio study J. Mol. Graph. Model. 92 296–302
[36] Azam S et al 2019 DFT study of the electronic and optical properties of ternary chalcogenides AlₓTe₄ Mater. Res. Express 6 116314
[37] Irfan M et al 2019 DFT simulations of optoelectronic and elastic features of cubic samarium zirconate (Sm₂Zr₂O₇) Comput. Condens. Matter 21 c00414
[38] Dressel M and Gruener G 2002 Electrodynamics of Solids: Optical Properties of Electrons in Matter. (UK: Cambridge University Press)
[39] Azam S, Goumri-Said S, Khan S A and Kanoun M B 2019 Electronic, optical and thermoelectric properties of new metal-rich homological selenides with palladium–indium: density functional theory and Boltzmann transport model J. Phys. Chem. Solids 109 229