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Research Article

First-principles Calculations of $TlCdF_3$ Compound under Pressure

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ABSTRACT

The present study focused on investigating various properties including structural, elastic, electronic, and optical of $TlCdF_3$ compound under hydrostatic pressure using Density Functional Theory (DFT). The estimated results were consistent with previous investigations. The analysis of the electronic band structures between 0 and 50 GPa revealed that this compound possesses an indirect band gap. The stress-strain method was used to explain elastic properties, and the findings revealed that this compound is ductile, anisotropic and mechanically stable between 0 and 50 GPa. Investigations were done on significant optical features such as refractive index n (ω), extinction coefficient k (ω), absorption coefficient α (ω) and reflectivity R (ω) at various pressures between 0 and 50 eV. Our results imply that $TlCdF_3$ compound has the potential for a broad range of technological applications under hydrostatic pressure.

1. Introduction

The technical and scientific significance of fluoride-type perovskite materials (XYF_3) has been probed due to their various applications in optoelectronic, medical field, magnetism, semi-conductivity, transistors, memory storages devices, light-emitting devices, catalysis [1-5]. Researchers are becoming more and more interested in these kinds of ternary compounds owing to their electronic, optical, thermodynamical, elastic, and vibrational properties [1-8].

XYF_3, where X (X = alkali metal) and Y (Y = transition metal or alkaline metal) elements represent cations and F (fluorine) elements express an anion, is the standard chemical formula for the well-known alloys as fluoro-perovskites [1]. Herein, we selected $TlCdF_3$ fluoro-perovskite compound as they can be potential candidates for technological applications due to their wide band gap value. This compound has been studied both theoretically [7-9] and experimentally [10-13] so far. Zaman et al. [14] also theoretically reported physical properties of $TlCdCl_3$ and $TlCaCl_3$ compounds within WIEN2k code in the space group Pm-3m. They found that these compounds exhibit wide and indirect band gap characteristics. Using DFT within GGA+U approximations, the electronic, optical, and elastic characteristics of $TlCaF_3$, $TlCdF_3$, $TlHgF_3$ and $TlMgF_3$ compounds were evaluated by Khan et al. [7]. They stated that these compounds show a ductile nature. By employing WIEN2k code for first principles calculation, Cheriet et al. [8] conducts a theoretical analysis of the physical properties of the title compound. Their research indicates that the band gap value for $TlCdF_3$ compound was determined as 3.66 eV for WC approach and 5.70 eV for TB-mBJ method. First-principles calculation utilizing TB-mBJ approximation of $TlCaF_3$ and $TlCdF_3$ compounds were predicted by Sohail et al. [9].

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Chabin et al. [10] experimentally reported the thermal properties of $TlCdF_3$ compound. Rousseau et al. [11] experimentally investigated the phase transition of the title compound using Raman Scattering. The third and fourth elastic constants of $TlCdF_3$ compound were experimentally researched by Ref. [12]. The elastic constants of $TlCdF_3$ compound were studied by Berger et al. [13] via Brillouin scattering. Fujimoto et al. [6] were experimentally exploring the luminescence as well as scintillation properties of $TlMgCl_3$ compound using the Bridgman–Stockbarger method. They indicate that $TlMgCl_3$ compound have a great potential for Gamma-ray and X-ray application due to this compound's high atomic number and medium density.

In spite of all the effort, the research on how pressure dependence of physical properties of $TlCdF_3$ compound is quite restricted. Hence, this study has been attempted to be clarified to serve as a guide for future research. The study is structured as follows: Following the introduction, the second section elaborates on our computational method. The examined structural, elastic, electronic and optical results are given in the third section. Finally, the conclusion part presents a summary of the findings.

2. Computational Methods

In the present study, VASP [15-17] (Vienna Ab initio Simulation Package) code was employed for performing the calculations. VASP is a widely used computational tool that operates within the framework of density functional theory (DFT) and employs the projector augmented wave (PAW) method [18] for treating electron-ion interactions. The Perdew-Burke-Ernzerhof (PBE) [19] functional, which is a generalized gradient approximation (GGA) for the exchange-correlation energy, was utilized to handle the electronic interactions. The PBE functional has been proven to provide reliable results for a variety of materials and properties. To ensure convergence of the calculations, a convergence test was conducted. Following the convergence test, the number of k-points was fixed to 16x16x16 in the Monkhorst-Pack [20] scheme, with a 700 eV cut-off energy. For the electronic band calculations, which require higher precision, the number of k-points was increased to 32 x 32 x 32. This increased density of k-points allows for a more accurate determination of the electronic band structure. By employing these computational parameters and methods, the study aimed to predict reliable and accurate results for investigating properties of the $TlCdF_3$ compound under hydrostatic pressure.

3. Results and Discussion

3.1. Structural properties under pressure

$TlCdF_3$ compound lattice parameters are obtained with the use of fully geometrical relaxation. In the equilibrium structure, Tl atom (0.00, 0.00, 0.00), Cd atom (0.50, 0.50, 0.50) and F atoms (0.00, 0.50, 0.50), (0.50, 0.00, 0.50) and (0.50, 0.50, 0.00) are placed in Wyckoff positions. Table 1 displays the lattice constant (a_0) values calculated within GGA-PBE. The computed lattice constant of this compound is found as 4.477 Å at zero pressure. It agrees well with the experimental lattice constant of 4.395 Å stated in Ref [11]. Table 1 also indicates how lattice constant changes as pressure rises. It is obvious that it gets smaller with increasing pressure.

Table 1. Lattice constant values a_0 **(Å)** at different pressures for $TlCdF_3$ compound

Pressure	Present a_0 (Å)	Exp. a_0 (Å)	Theory a_0 (Å)
0 GPa	4.477	4.395 [11]	4.49 [7] 4.492^{PBE} [8] 4.402^{WC} [8] 4.325^{LDA} [8] 4.33 [9]
10 GPa	4.296		
20 GPa	4.183		
30 GPa	4.099		
40 GPa	4.035		
50 GPa	3.981		

3.2. Elastic properties under pressure

Investigation of pressure-induced elastic properties provides a powerful tool to describe atomic bonding, mechanical stability, phase transformation, hardness and intrinsic characteristics of the material which helps in the understanding and attraction of their future applications. Herein, the elastic constants (C_{ij}) of $TlCdF_3$ compound were computed by the "stress-

strain" method [21] in the pressure range of 0-50 GPa. The obtained results are tabulated in Table 2 at 0 GPa and 0 K. It is worth noting that our results are quite consistent with the experimental values [11, 13] of C_{11}=102.8 (103.6) GPa, C_{12}=38.5 (39.6) GPa and C_{44}=17.7 (18.08) GPa, respectively. These results also agree generally with earlier theoretical reports [7-9].

At the analyzed pressures, the elastic constants of $TlCdF_3$ compound are positive. With the following conditions, we can say that this compound satisfies the requirements for mechanical stability [22]: $C_{11}>0$; $C_{44}>0$; $(C_{11}+2C_{12})>0$; $(C_{11}-C_{12})>0$. As shown in Fig. 1a, the elastic constants C_{11} and C_{12} climb linearly with increasing pressure, whereas C_{44} decreases.

The Voigt-Reuss-Hill approximation [23-25] was used to clarify the important elastic parameters including bulk modulus (B), Young's modulus (E), shear modulus (G), and Poisson's ratio (ν) of $TlCdF_3$ compound. The equations used in the calculations are given below [26-28]:

$$B_V = B_R = B_H = \frac{C_{11}+2C_{12}}{3} \quad (1)$$

$$G_H = \frac{G_V+G_R}{2} \quad (2)$$

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

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

$$E = \frac{9B_HG_H}{3B_H+G_H} \quad (5)$$

$$\nu = \frac{3B_H-2G_H}{6B_H+2G_H} \quad (6)$$

Table 2 contains a list of these findings, and Figs. 1(b-d) show the pressure dependence graphs. According to Fig. 1b, the bulk modulus increases with pressure more than Young's and Shear modulus. Cauchy pressure (C_{12}-C_{44}), B/G ratio and Poisson's ratios (ν) are three important markers for predicting a material's ductility or brittleness. The material is a classified ductile if the B/G ratio [27, 29] is more than 1.75, the Poisson's ratio is bigger than 0.26 [14, 30], and the Cauchy pressure [27, 31] is positive; otherwise, it is considered brittle. The title compound is ductile, as shown by our findings. These results corroborate with those of other studies [7-9]. Furthermore, as shown in Fig. 1c, the increase in B/G ratio with pressure demonstrates that the ductility of the material increases.

Table 2. Calculated elastic properties of $TlCdF_3$ compound at 0 GPa with other results

$TlCdF_3$	Present	Other	Exp.
C_{11} (GPa)	110.556	106.62 [7] 124.7 [8] 114.34 [9]	102.8 [11] 103.6 [13]
C_{12} (GPa)	35.761	46.89 [7] 39.59 [8] 32.57 [9]	38.5 [11] 39.6 [13]
C_{44} (GPa)	13.352	18.09 [7] 11.53 [8] 15.08 [9]	17.7 [11] 18.08 [13]
Cauchy Pressure (GPa)	22.409		
B (GPa)	60.693	66.80 [7] 67.99 [8] 172.03 [9]	
G (GPa)	20.473	22.13 [7] 20.109 [8] 22.78 [9]	
E (GPa)	55.210	59.81 [7] 54.912 [8] 72.631 [9]	
B/G	2.965	3.01 [7] 3.380 [8] 7.549 [9]	
ν	0.348	0.50 [7] 0.365 [8] 0.43 [9]	
A	0.357	0.60 [7] 0.8629 [8] 0.369 [9]	

The degree of elastic anisotropy in materials is calculated using the Zener anisotropy factor [26-28]:

$$A = \frac{2C_{44}}{C_{11}-C_{12}} \quad (7)$$

The anisotropy factor has a value of 1 for entirely isotropic materials [9, 14]. It was found to be 0.357 at 0 GPa for this compound. According to our obtained values, the title compound shows anisotropic behavior in the 0-50 GPa pressure range. As shown in Fig. 1d, Zener anisotropy factor diminishes linearly as pressure rises.

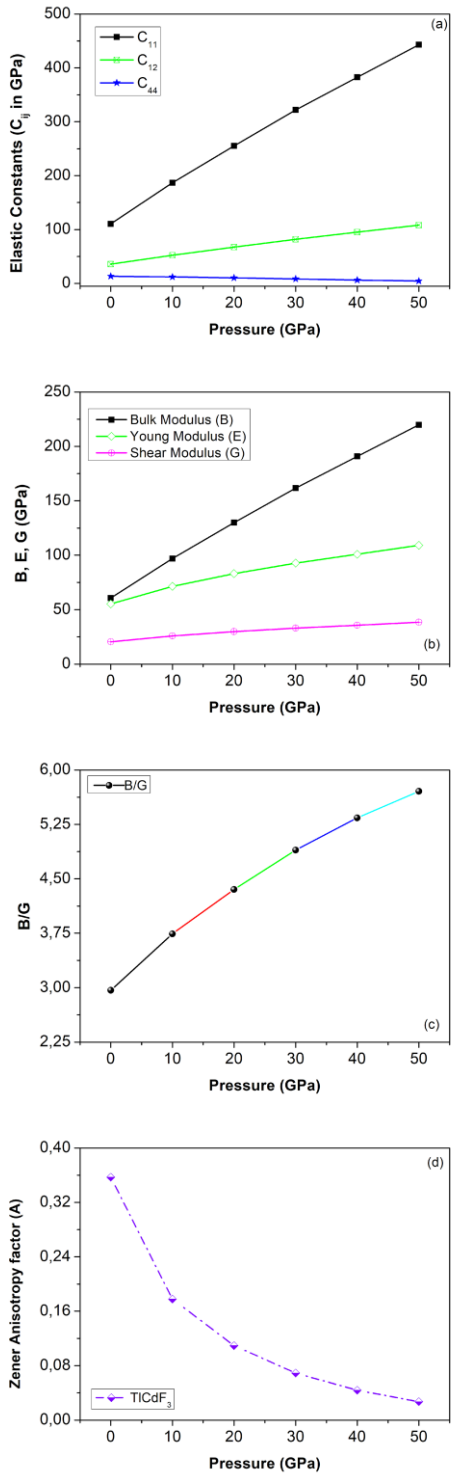

Figure 1. a) Elastic constants (C_{ij}), b) Bulk, Shear, and Young's moduli, c) B/G ratio, and d) Zener anisotropy factor variations with pressure for $TlCdF_3$ compound

3.3. Electronic properties under pressure

Using the equilibrium lattice constants of $TlCdF_3$ compound, the electronic band structures and partial density state (PDOS) corresponding to high symmetry directions were calculated under pressure. Since the electronic band gap characteristic of $TlCdF_3$ compound is the same at all pressure levels (0-50 GPa), Figs. 2 (a-b) displays graphs for 0 GPa and 50 GPa pressure. The conduction band minimum is situated at the X high symmetry point, while the valence band maximum is located at the R high symmetry point, as shown in Figs. 2. As a result, the indirect band gap of this compound at 0 GPa is 3.817 eV. $TlCdF_3$ compound indirect band gap values at 10 GPa, 20 GPa, 30 GPa, 40 GPa, and 50 GPa are 3.577 eV, 3.345 eV, 3.122 eV, 2.927 eV, and 2.749 eV, respectively.

Khan et al. [7] is reported that $TlCdF_3$ compound has an indirect band gap because the valence band maximum is at M symmetry point and the conduction band minimum occurs at Γ symmetry point. Their calculated energy band gap is 3.46 eV at 0 GPa using the GGA+U. According to Cheriet et al. [8], the top of the valence band is at the M-point, while the bottom of the conduction band is at the X-point, with an indirect band gap of 5.70 eV for TB-mBJ and 3.66 eV for WC approximation. Sohail et al. [9] found that title compound has a direct band gap at X symmetry point with 5.7 eV using the TB-mBJ potential method. Unfortunately, no experimental studies on the electronic band structure of $TlCdF_3$ compound are currently available to analyze and debate the findings. The obtained results at various pressures present in Table 3 and contrasted with findings from earlier theoretical investigations [7, 9]. As can be seen in Table 3, very consistent results were achieved at 0 GPa.

The electronic partial density of states (PDOS) is the energy levels occupied by the electrons of each atom or group of atoms in a material. In Fig. 2a, on the right side, it is shown that the F atom contributes most to the valence band between 0 and -5 eV. The Cd atom primarily contributes to the valence band between -5 and -10 eV. Additionally, the Tl atom makes a larger contribution to the total density of states in the conduction band. This information can be used to gain insights into the electronic properties of the material and to design materials with specific electronic properties for various applications

Table 3. Energy band gap values (E_g, in eV) of $TlCdF_3$ compound at various pressures

	Theory	Present					
	0 GPa	**0 GPa**	**10 GPa**	**20 GPa**	**30 GPa**	**40 GPa**	**50 GPa**
E_g^{M-M}	5.21 [7] 5.24 [9]	5.18	4.98	4.48	4.41	5.85	4.18
E_g^{X-X}	3.67[7] 5.7 [9]	4.27	4.28	4.14	4.19	4.10	4.12
$E_g^{\Gamma-\Gamma}$	3.46 [7] 6.94 [9]	5.92	7.23	9.04	8.95	9.50	10.18
$E_g^{R-\Gamma}$	6.19 [7] 5.82 [9]	4.44	4.98	5.67	5.72	6.02	6.00
$E_g^{\Gamma-X}$	3.23[7] 6.69[9]	5.26	5.82	6.44	6.45	6.62	6.87

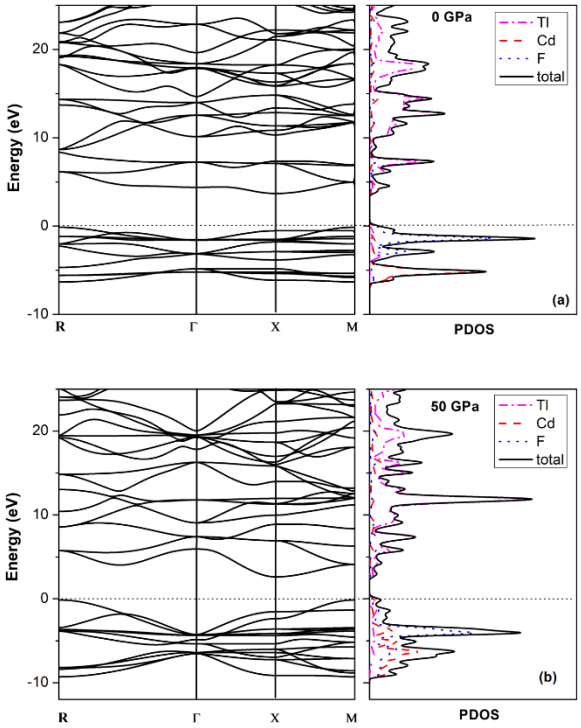

Figure 2. Computed electronic band structure and partial density of states (PDOS) of $TlCdF_3$ compound at a) 0 GPa and b) 50 GPa

3.4. Optical properties under pressure

The complex dielectric function, represented by $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$, provides detailed information about the linear optical characteristics of a material [9, 32-34]. The optical features of $TlCdF_3$ compound have been investigated under various pressures and energies (0–50 eV). The curves of real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ parts of dielectric function of our investigated compound are shown in Figs. 3(a-b). The pressures are shown in steps of 10 GPa from 0–50 GPa.

The static dielectric constant represents the value of $\varepsilon_1(\omega)$ at zero energy ($\omega = 0$). For $TlCdF_3$ at 0 GPa, $\varepsilon_1(0)$ is found to be approximately 2.94, while at 50 GPa, it increases to around 3.52. This indicates that an increase in pressure leads to a higher static dielectric constant. The imaginary part of the dielectric function, $\varepsilon_2(\omega)$, exhibits peaks at specific energy values. For $TlCdF_3$, the largest peaks of $\varepsilon_2(\omega)$ are detected at 5.27 eV at 0 GPa and 7.9 eV at 50 GPa in the ultraviolet (UV) region (3.1-124 eV). The imaginary $\varepsilon_2(\omega)$ parts of the dielectric function show that the maximum peak values rise with pressure.

With the use of the Kramer-Kronig relations [7, 9, 14, 33], the refractive index n (ω), extinction coefficient k (ω), absorption coefficient α (ω), and reflectivity R (ω) of $TlCdF_3$ compound are calculated and depicted in Figs. 4 (a-d). The curves shapes for refractive index n (ω) and extinction coefficient k (ω) follow the same pattern as the real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ parts of the complex dielectric function, respectively. The static refractive index of $TlCdF_3$ compound at 0 GPa is found to be 1.71. As the pressure increases to 50 GPa, the static refractive index also increases and becomes 1.88. The main peak value of the extinction coefficient increases with pressure. The static reflectivity R (0) also rises as the pressure increases. This indicates that the material becomes more reflective with increasing pressure.

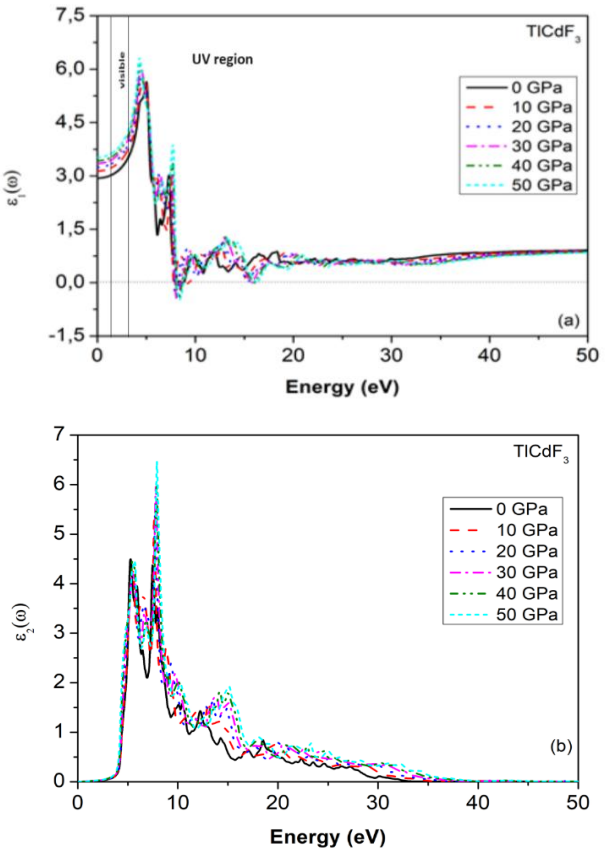

Figure 3. a) Real part of dielectric function $\varepsilon_1(\omega)$, b) imaginary part of dielectric function $\varepsilon_2(\omega)$ of $TlCdF_3$ compound

The absorption coefficient denotes the quantity of energy lost by the wave as it goes across the material. The incident photons in the ultraviolet region have energies ranging from 3.1 eV to 124 eV [9, 34]. As shown in Figure 4c, the absorption spectra show the peak starting UV region. It is noticeable that the absorption coefficient curves shift to higher energies with the increase in pressure. This implies that the optical features of $TlCdF_3$ compound become more pronounced and enhanced under higher pressures. As a result, this material has the potential to be used in optoelectronic devices operating in the ultraviolet region under pressure (0-50 GPa). The current optical results of $TlCdF_3$ compound are consistent with previous research [7, 9]. This agreement adds confidence to the accuracy and reliability of the investigation.

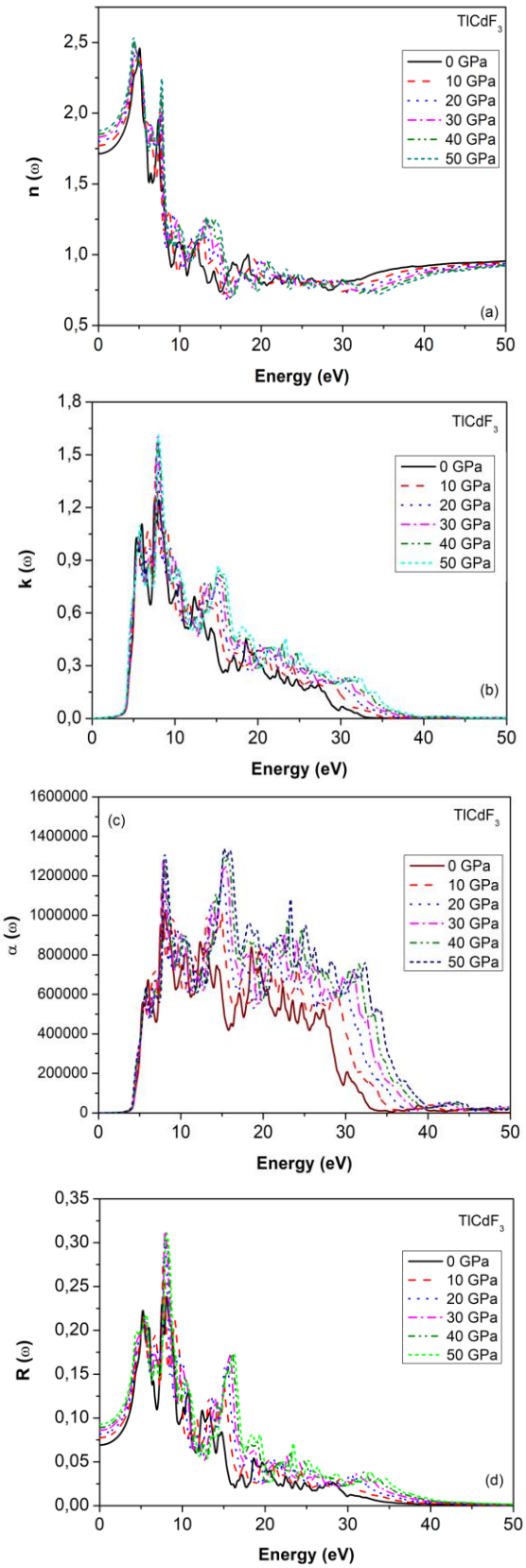

Figure 4. The optical properties of $TlCdF_3$ compound under pressure

4. Conclusion

GGA-PBE approximation is used to evaluate the first principles calculation of the $TlCdF_3$ fluoro-perovskites compound at various pressures. Our

calculated ground state properties, electronic band structure, optic, elastic constants and related properties agree with literature. $TlCdF_3$ compound exhibits an indirect band gap under investigated pressures, in accordance with the electronic band structure. This compound is ductile and mechanically stable up to 50 GPa, as evidenced by its elastic characteristics. The various optical properties are also investigated across a broad energy range of 0 eV to 50 eV. It is found that $TlCdF_3$ exhibits absorption in the UV energy range. Due to these properties, $TlCdF_3$ compound can be suitable for technological application for the fluoro-perovskite family. These results can also give valuable information for researchers exploring new materials in the fields of semiconductors, optics, and engineering materials.

Article Information Form

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Authors' Contribution
B.K.: Writing-original draft, Investigation, Calculations, Visualization, Conceptualization, Review & editing. **Y.O.C:** Calculations, Conceptualization, Writing – review & editing.

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No conflict of interest or common interest has been declared by the authors.

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References

[1] M. K. Shahzad, S. Hussain, M. U. Farooq, R. A. Laghari, M. H. Bilal, S. A. Khan, M. Tahir, A. Khalil, J. U. Rehman, M. M. Ali, "First-principles calculations to investigate structural, electronic, elastic and optical properties of radium based cubic fluoro-perovskite materials," Heliyon, vol. 9, pp. E13687, (2023).

[2] Shakeel, A. H. Reshak, S. Khan, A. Laref, G. Murtaza, J. Bila, "Pressure induced physical variations in the lead free fluoropervoskites XYF_3 (X=K, Rb, Ag; Y=Zn, Sr, Mg): Optical materials," Optical Materials, vol. 109, pp. 110325, 2020.

[3] T. Tianyu, Y. Tang, "First-Principles Calculations to Investigate Direct-Band Novel Cobalt-Based Double Perovskite Materials for Optoelectronic Applications, " Energy & Fuels, vol. 37, pp. 1266−1274, 2022.

[4] J. Saddique, M. Husain, N. Rahman, R. Khan, Zulfiqar, A. Iqbal, M. Sohail, S. A. Khattak, S. N. Khan, A. A. Khan, A.H. Reshak, A. Khan, "Modeling structural, elastic, electronic and optical properties of ternary cubic barium based fluoroperovskites $MBaF_3$ (M = Ga and In) compounds based on DFT," Materials Science in Semiconductor Processing, vol. 139, pp. 106345, 2022.

[5] T. Nishimatsu, N. Terakubo, H. Mizuseki, Y. Kawazoe, D. A. Pawlak, K. Shimamura,

T. Fukuda, "Band Structures of Perovskite-Like Fluorides for Vacuum-Ultraviolet-Transparent Lens Materials," Japanese Journal of Applied Physics, vol. 41, pp. 090301, 2002.

[6] Y. Fujimoto, M. Koshimizu, T. Yanagida, G. Okada, K. Saeki, K. Asai, "Thallium magnesium chloride: A high light yield, large effective atomic number, intrinsically activated crystalline scintillator for X-ray and gamma-ray detection," Japanese Journal of Applied Physics, vol. 55, pp. 090301, 2016.

[7] S. Khan, S. U. Zaman, R. Ahmad, N. Mehmood, M. Arif, H. J. Kim, "Ab Initio Investigations of Structural, Elastic, Electronic and Optical Properties of the Fluoroperovskite $TlXF_3$ (X = Ca, Cd, Hg, and Mg) Compounds," Materials Research Express, vol. 6, no.12, pp. 125923, 2020.

[8] A. Cheriet, B. Lagoun, M. Halit, M. Zaabat, C. Abdelhakim, H. Lidjici, "First-principles study of structural, electronic, optical and elastic properties of cadmium based Fluoro-Perovskite $MCdF_3$ (M= Rb, Tl)," Solid State Phenomena, vol. 297, pp. 173-186, 2019.

[9] M. Sohail, M. Husain, N. Rahman, K. Althubeiti, M. Algethami, A. A. Khan, A. Iqbal, A. Ullah, A. Khanfg, R. Khan "First-principal investigations of electronic, structural, elastic and optical properties of the fluoroperovskite $TlLF_3$ (L= Ca, Cd) compounds for optoelectronic applications," RSC Advances, vol. 12, no.12, pp. 7002-7008, 2022.

[10] M. Chabin, F. Gilletta, C. Ridou, "Thermal properties of $TlCdF_3$ and $RbCaF_3$ near their phase transitions," Physica status solidi (a), vol. 48(1), pp. 67-70, 1978.

[11] M. Rousseau, J. Y. Gesland, J. Julliard, J. Nouet, J. Zarembowitch, A. Zarembowitch, "Crystallographic, elastic, and Raman scattering investigations of structural phase transitions in $RbCdF_3$ and $TlCdF_3$," Physical Review B, vol. 12, no.4, pp.1579, 1975.

[12] M. Fischer, "Third and fourth order elastic constants of fluoperovskites $CsCdF_3$, $TlCdF_3$, $RbCdF_3$, $RbCaF_3$," Journal of Physics and Chemistry of Solids, vol. 43, no.8, pp. 673-682, 1982.

[13] J. Berger, G. Hauret, M. Rousseau, "Brillouin scattering investigation of the structural phase transition of $TlCdF_3$ and $RbCaF_3$," Solid State Communications, vol. 25, no.8, pp. 569-571, 1978.

[14] S. U. Zaman, N. Rahman, M. Arif, M. Saqib, M. Husain, E. Bonyah, Z. Shah, S. Zulfiqar, A. Khan, "Ab initio investigation of the physical properties of Tl based chloroperovskites $TlXCl_3$ (X= Ca and Cd)," AIP Advances, vol. 11(1), pp. 015204, 2021.

[15] J. Hafner, "Ab-initio simulations of materials using VASP: Density-functional theory and beyond," Journal of Computational Chemistry, vol. 29, pp. 2044-2078, 2008.

[16] G. Kresse, J. Hafner, "Ab initio molecular-dynamics simulation of the liquid-metal–amorphous semiconductor transition in germanium," Physical Review B, 49: pp.14251, 1994.

[17] G. Kresse, J. Hafner, "Ab initio molecular dynamics for liquid metals," Physical Review B, vol.47, pp. 558-561, 1993.

[18] G. Kresse, J. Furthmuller, "Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set," Computational Materials Science, vol. 6, pp. 15-50, 1996.

[19] J. P. Perdew, K. Burke, M. Ernzerhof, "Generalized gradient approximation made simple," Physical Review Letters, vol. 77, pp. 3865-3868, 1996.

[20] H. J. Monkhorst, J. D. Pack, "Special points for Brillouin-zone integrations,"

Physical Review B, vol. 13, no. 12, pp. 5188-5192, 1976.

[21] Y. Le Page, P. Saxe, "Symmetry-general least-squares extraction of elastic data for strained materials from ab initio calculations of stress," Physical Review B, vol. 65 10, pp. 104104, 2002.

[22] F. Mouhat, F. X. Coudert, "Necessary and sufficient elastic stability conditions in various crystal systems," Physical Review B, vol. 90, pp 224104, 2014.

[23] A. Reuss, "Berechnung der Fließgrenze von Mischkristallen auf Grund der Plastizitätsbedingung für Einkristalle", Zeitschrift für Angewandte Mathematik und Mechanik, vol. 9, pp. 49. 1929.

[24] W. Voigt, "Lehrbuch der Kristallpysik", vol. 34, Teubner, Leipzig, Germany, 1928.

[25] R. Hill, "The Elastic Behaviour of a Crystalline Aggregate," Proceedings of the Physical Society, Section A, vol. 65, pp. 349, 1952.

[26] V. V. Bannikov, I. R., Shein, A. L. Ivanovskii, "Elastic properties of antiperovskite-type Ni-rich nitrides $MNNi_3$ (M= Zn, Cd, Mg, Al, Ga, In, Sn, Sb, Pd, Cu, Ag and Pt) as predicted from first-principles calculations," Physica B: Condensed Matter, vol. 405 (22), pp.4615-4619, 2010.

[27] T. Seddik, R. Khenata, O. Merabiha, A. Bouhemadou, S. Bin-Omran, D. Rached, "Elastic, electronic and thermodynamic properties of fluoro-perovskite $KZnF_3$ via first-principles calculations," Applied Physics A, vol. 106, pp. 645-653, 2012.

[28] B. Mayer, H. Anton, E. Bott, M. Methfessel, J. Sticht, J. Harris, P. C. Schmidt, "Ab-initio calculation of the elastic constants and thermal expansion coefficients of Laves phases," Intermetallics, vol. 11(1), pp. 23-32, 2003.

[29] S. F. Pugh, "XCII. Relations between the elastic moduli and the plastic properties of polycrystalline pure metals," The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, vol. 45 (367), pp. 823-843, 1954.

[30] I. N. Frantsevich, F. F. Voronov, S. A. Bokuta, "Elastic Constants and Elastic Moduli of Metals and Insulators Handbook", edited by I. N. Frantsevich Naukuva Dumka, Kiev, 1982.

[31] D. G. Pettifor, "Theoretical predictions of structure and related properties of intermetallics," Materials science and technology, vol. 8, pp. 345-349, 1992.

[32] M. Fox, "Optical Properties of Solids", Oxford University Press, New York, 2001.

[33] W. Belkilali, F. Belkharroubi, M. Ameri, N. Ramdani, F. Boudahri, F. Khelfaoui, A. Amara, S. Azzi, L. Drici, I. Ameri, Y. Douri, "Theoretical investigations of structural, mechanical, electronic and optical properties of NaScSi alloy," Emergent Materials, vol. 4, pp. 1465-1477, 2021.

[34] M. A. Iqbal, N. Erum, "Opto-Electronic Investigation of Rubidium Based Fluoro-Perovskite for Low Birefringent Lens Materials," Scientific Inquiry and Review, vol. 1(1), pp. 37-48, 2017.