Investigations of physical properties of lithium-based chalcopyrite semiconductors: non-toxic materials for photovoltaic applications

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The ab-initio calculations have been executed for structural, electronic and optical properties of $LiAlTe_2$, $LiGaTe_2$ and $LiInTe_2$ chalcopyrite structured solids and these calculations are grounded on the principle of density functional theory employed into the full potential augmented plane wave method. The computed lattice constants oscillating from a = 6.257 Å to 6.450 Å and c = 12.044 Å to 12.256 Å for $LiXTe_2$ (X=Al, Ga and In) and also these values consistent with experimentally existed lattice constants. From the study of electronic band-gap, it confirms that these compounds are good semiconductors with direct band-gaps from 2.22 eV, 1.48 eV and 1.61 eV for $LiXTe_2$ (X=Al, Ga and In). The result of optical properties confirms that these chalcopyrite semiconductors can be the fortunate compounds for the photovoltaic applications.

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1. Introduction

From a century, the group of chalcogenides having tetragonal symmetry have been investigated, still they attract the interest of researchers because of their favourable solid-state properties i.e., structural, electronic, elastic, optical [1-2]. These compounds are reliable in the photonic, electronic, and optoelectronic fields, they are having the superb linear and non-linear optical properties also they are majorly useful in photovoltaic cells, detectors, LEDs, lasers, modulators, diodes, optical light eliminators [3-4]. The chalcopyrite materials are promising candidates for solar cells and several intricate potential applications [5]. Generally, this type of compound are semiconductors with narrow and direct band gaps (1 eV to 3 eV), which is the main condition in manufacturing the highly efficient photovoltaic cells due to their great capacity to absorb visible light spectrum in the electromagnetic spectrum. These compounds of type $A^{I}B^{III}C^{VI}_2$configures into the tetragonal structure with the space group of I-42d and co-ordination no. 4 [6]. In this tetragonal structure every atom allied with the neighbour atoms (4), 'C' is anion which is connected with two 'A' and two with 'B' which are cations whereas every cation allied with four anions which forms the above discussed tetragonal configuration. If we are looking towards energy crisis, only sun is the alternate resource of green energy because of its various features likewise: eco-friendly, zero emission, wellbeing feature, noiseless etc. The amount of energy emitted from the sun in an hour is this much that can accomplish the need of power for a year in all over the world thus we are trying to utilize the emitted energy from sun to resolve the power crisis universally. For improving the efficiency of the photovoltaics there are several efforts have been made which also includes the third-generation photovoltaic cells, an isolated intermediate band sandwiched among the valence and the conduction band of third-generation

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solar cells which is used in the transformation of electrons from valence band to the conduction band weather the transformation is direct or from intermediate band of semiconductor. But in the obsolete solar cells this transformation of electrons follows directly from the valence to the conduction band [7-8], they possess the efficiency of 63.1% and the single junction photovoltaic cells possess 40.7% after doing more improvements in the third-generation photovoltaics their efficiency reached at 86.8% by implementing the essential number of intermediate bands. Regarding the intermediate bands in multitude specimen there are lots of studies have done by experimentally and theoretically which can enhance the optical absorption [9]; there are numerous studied data reported regarding the chalcopyrite structured solids [10]. The chalcopyrite compounds having the wide band-gaps are potential candidate for thin film intermediate photovoltaic [11-16]. In semiconductor materials, the most important feature is the energy band gap due to which we get the critical peaks of absorption coefficient in the optical spectrum. Researchers are attracted towards the intermediate band because by doing the implementation of this band the energy band gap started increasing which is the favourable condition to attain the high solar energy adaptation efficiencies [17-19]. Now days, the ternary lithium-based chalcopyrite compounds are the centre of attraction for researchers and scientist because of their fabulous applications in the field of photovoltaics, detectors, modulators, optical oscillators, diodes etc. most of these compounds have narrow and direct energy band gaps. Ma ***et al.*** [19] have reported the detailed study of $LiInSe_2$ and $LiInTe_2$ chalcopyrites and they reported that these compounds having the direct band gap 1.684 eV for $LiInSe_2$ and 1.313 eV for $LiInTe_2$. According to him, these are good for the application in the solar cells. Kosobutsky ***et al.*** [20] have been performed the ab initio calculations for the phonon spectra and DoS of the 'Li' containing chalcopyrite solid crystals. Ma ***et al.*** [21] have reported the first principles study of the $LiGaS_2$ and $LiGaSe_2$ chalcopyrites. They reported that these compounds having direct band gap, 3.12 eV for $LiGaS_2$ and 2.34 eV for $LiGaSe_2$ respectively. Also, they reported that these compounds are potential candidate for mid-IR region. Kong ***et al.*** [22] have reported the DFT calculations for $LiInS_2$ and $LiInSe_2$ and suggested that these compounds having direct band gap and they are reliable for the photovoltaic applications. In the manufacturing of novel photovoltaic devices containing the chalcopyrite semiconductors need enhance information about their electronic and optical features. From the above-mentioned literatures, we can say that numerous studied have been done related to the structural, electronic, optical properties of Li- based ternary compounds by implementing the density functional theory. In this research work we are looking towards the importance of chalcopyrite semiconductors and performed ab-initio calculations for structural, electronic and optical properties of $LiAlTe_2$, $LiGaTe_2$ and $LiInTe_2$ chalcopyrite compounds by using the concept of density functional theory. This study will be beneficial for understanding the structural and physical properties of $LiXTe_2$ (X=Al, Ga, Te); which can be the potential materials for the photoelectric devices. The outline of this research paper is as follows: In Section 2, we have been given the short description of computational method used for the calculations, discussions of results about the structural, electronic and optical properties are given in Section 3, whereas summary and conclusion are described in the last Section 4.

2. Computational methods

Regarding the understanding of structural, electronic and optical properties of the chosen chalcopyrite compounds, we performed the first principles calculations within the framework of density functional theory with the help of using Full Potential Linearized Augmented Plane Wave (FP-LAPW) scheme [23-24] which is employed in the WIEN2K simulation package. For a unit cell the Kohn Sham equation [25] have been resolved in LAPW method. Here, l_{max} represents the atomic sphere extension of spherical harmonics and have been taken 10, the RK_{max} have been taken 7, here (RK_{max} is the multiplication of R_{MT} and K_{max}), here the R_{MT} defines minimum muffin tin radii of the atoms in compound's unit cell and the maximum modulus of the reciprocal vector in the first Brillouin zone representing by the K_{max}, the value of G_{max} have taken 12, here G_{max} represents the magnitude of the largest vector in fourier expansion of the charge density. The cut-off energy has been taken -6.0 Rydberg. The R_{MT} have been taken 1.97, 2.21, 2.32, 2.45 and 2.50

a.u for Li, Al, Ga, In and Te correspondingly. These muffin-tin radii are choosing in such kind of pattern that no drip of charge from muffin tins is corroborated. We have used the LSDA [26], PBE-GGA [27], PBEsol [28] and Wu-Cohen (WC-GGA) [29] exchange correlation potentials for the optimization of the structure i.e., the computation of lattice parameters and for the calculation of band-gaps and the band structure of the chosen compounds as well as for the SCF calculations. We get the accurate values of the lattice parameters by using LSDA potential. Also, we observe that the calculated band-gaps by using LSDA having good agreement with experimentally calculated band gaps for these compounds. From the various study of research papers, we can say that the determination of accurate band-gap is a biggest task for all of us. Hence, the upcoming properties are depending on the accurate band-gap. So, we use the TB-mBJ method [30] with LSDA-GGA potential and we observed that from this approach we get the accurate band-gaps. The convergence criterion for energy and the charge disparity in consecutive repetitions of SCF cycles have been fixed to 10^{-5} Ry and $10^{-4}e$ respectively. For computing the structural, electronic and optical parameters, we have used the k-mesh 21 x 21 x 21.

3. Results and discussion

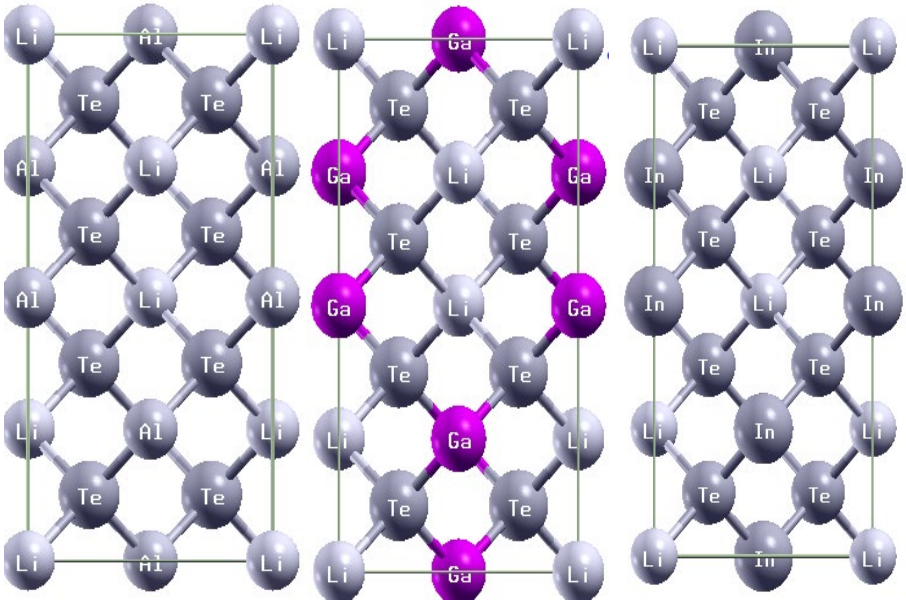
3.1. Structural Properties

The chosen ternary chalcopyrite compounds $LiXTe_2$ (X= Al, Ga, In) constitutes into the tetragonal crystal structure having the space group I-42d. In this geometry the Li-atom constituted up on the (0, 0, 0);(0, 1/2, 1/4), the Al, Ga, and In-atoms constituted up on the (1/2, 1/2, 0);(1/2, 0, 1/4) and the Te-atom constituted up on the (u, 1/4, 1/8);(-u, 3/4, 1/8);(3/4, u, 7/8);(1/4, -u, 7/8) positions correspondingly. The optimized structures of the compounds are shown in the Fig 1. The optimization curve of lattice parameters with respect to the total energy has been given in the Fig 2. for these compounds and the calculated lattice constants a and c in angstrom equated with the existing experimental outcomes, c/a ratio, bulk modulus (B), pressure derivative of bulk modulus (B′), volume at equilibrium (V_0) and total energy (E_0) are given in the Table 1. Here *a (in Å)* represents the lattice parameter along x and y-direction and in the z-direction the lattice parameter is 'c'. We have been used the total six values of c/a for each and every volume for accurate determination of the c/a ratio and the exact lattice constants. This phenomenon of optimization, based on the Murnaghan equation of state [31]; which is inbuilt in the WIEN2K package. From the Table 1, we observe that the calculated lattice constants in this study having good consistency with the experimental lattice constants also it confirms the tetragonal symmetry for these compounds.

Table 1. The optimized structural parameters compared with experimentally exited data of $LiXTe_2$ (X=Al, Ga, In) chalcopyrites.

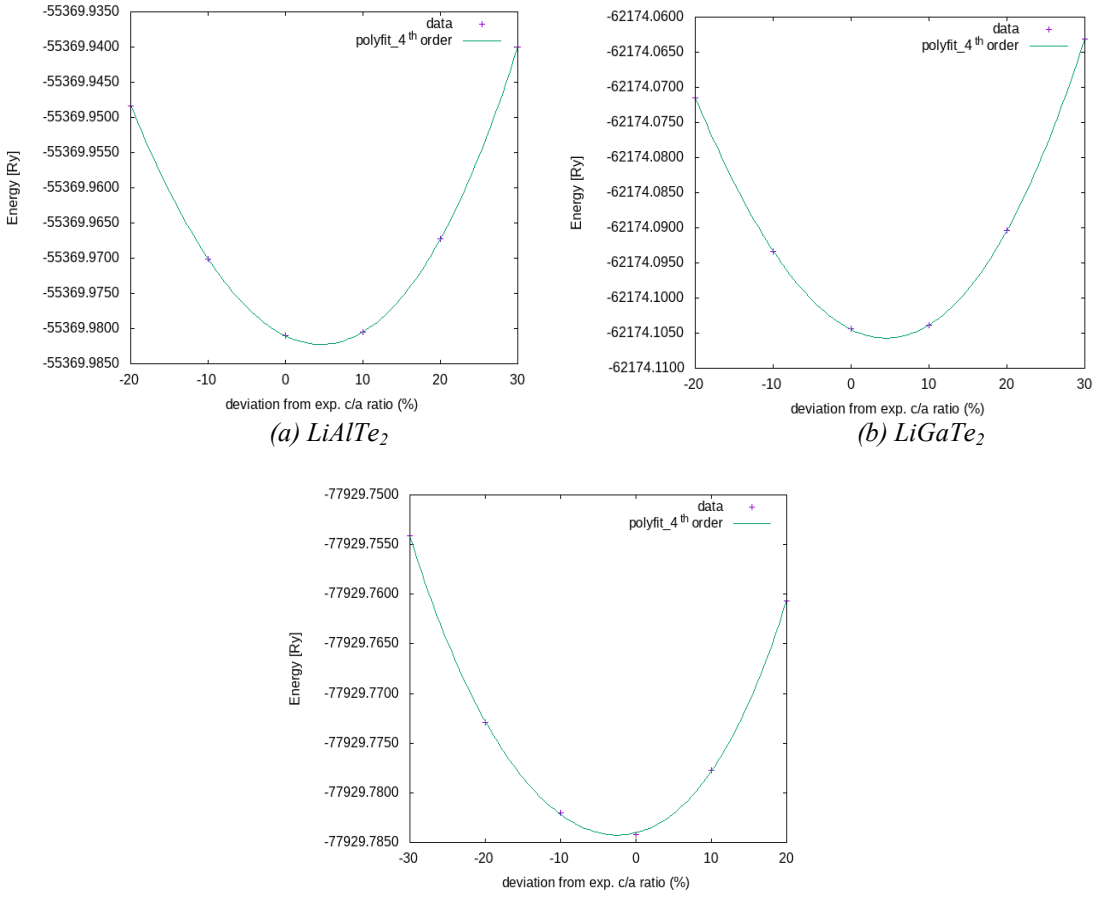
Compounds	**Lattice Constants (in *Å*)**		**Experimental (in *Å*)**		**c/a**	**B(*GPa*)**	**B′**	**V_0**	**E_0(*Ry*)**
	a	**c**	**a**	**c**					
$LiAlTe_2$	6.257	12.044	6.351[a]	11.691[a]	1.924	30.96	2.978	1544.642	-55369.971
$LiGaTe_2$	6.236	12.032	6.329[b]	11.682[b]	1.929	29.65	2.581	1556.189	-62174.095
$LiInTe_2$	6.450	12.256	6.398[c]	12.460[c]	1.899	28.46	2.483	1814.379	-77929.781

[(a)] Ref [36], [(b)]Ref [37] and [(c)]Ref [38].



(a) $LiAlTe_2$ *(b) $LiGaTe_2$* *(c) $LiInTe_2$*

Fig. 1. Crystal structure of $LiXTe_2$ (X=Al, Ga and In) compounds.



(a) $LiAlTe_2$ *(b) $LiGaTe_2$*

(c) $LiInTe_2$

Fig. 2. Optimization curve of lattice constants as a function of total energy for $LiXTe_2$ (X = Al, Ga and In) compounds.

3.2. Electronic Properties

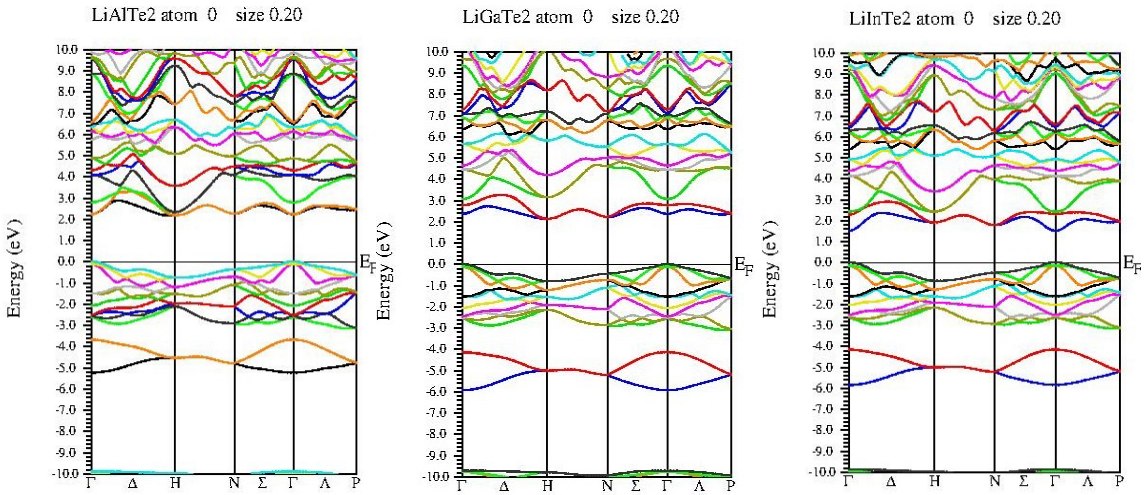
3.2.1. Bandgap, Band Structure and Density of States

We have been calculated the electronic properties of $LiXTe_2$ (X= Al, Ga and In) compounds by doing the computation of electronic band structure curves along with the computation of density of states (TDOS and PDOS). From the study of previous research work [32-35], we have observed that the chalcopyrite structured compounds possess direct band gap lies on the Γ_v-Γ_c point. In this study we obtain that these three compounds namely $LiAlTe_2$, $LiGaTe_2$ and $LiInTe_2$ having direct band gaps. Calculated band structures are shown in figure 3. From the band structure curves, we have seen that the maxima of valence band sited on Γ_v point in the valence band region and minima of conduction band sited on Γ_c point in the conduction band region since they are direct band gap semiconductor compounds. Calculated band gaps with available experimental data and data from the other studies are given in Table 2. From this table of calculated band gaps for the chosen compounds, we conclude that the results of LSDA potential having better agreement with the available data but for $LiGaTe_2$ (LGT) LSDA underestimates the band gap, so we have been employed the TB-mBJ method with LSDA potential and we got the band gap 2.137 eV for LGT we can say that this value closely agreed with the experimentally calculated band gap. Also, as per my knowledge, there is no experimental work have been performed for the calculation of electronic band gap of $LiAlTe_2$ (LAT) so we compare the calculated band gap for this compound with other's work and we have concluded that it is also have good agreement with other's work. The DoS plots for the mentioned ternary chalcopyrite semiconductor compounds are shown in the Figure 4. Figure 4 (a, b and c) represents the total density of states, Figure 4.1 (a, b, c, d, e and f) represents the partial density of states, Figure 4.1 (a, b and c) represents the contribution of atoms of the in d-state and Figure 4.1 (d, e and f) represents the contribution of atoms in s, p, d and f-states. At 0 eV we have been selected the Fermi level. Also, the valence band section has divided into two parts, in VB section the energy ranges from -3 eV to -6 eV the hybridization among the Al, Ga, and In-atoms is due to s-state and ranges from 0 eV to -3 eV, which is the nearest section to Fermi level the major input of the Al, Ga and In-atoms is due to p-states in this VB section the major contribution is due to the s-p hybridization. Energy ranges from 0 eV to 6 eV which is the conduction band section in this part the hybridization in between the Al, Ga and In-atoms due to the s and p-states or we can say that contribution in CB is due to the s-p hybridization. Also, Li and Te-atom have doing little contribution with d-state in the conduction band section.

Table 2. Calculated and experimental Band-gaps of $LiXTe_2$ (X=Al, Ga, In) chalcopyrites.

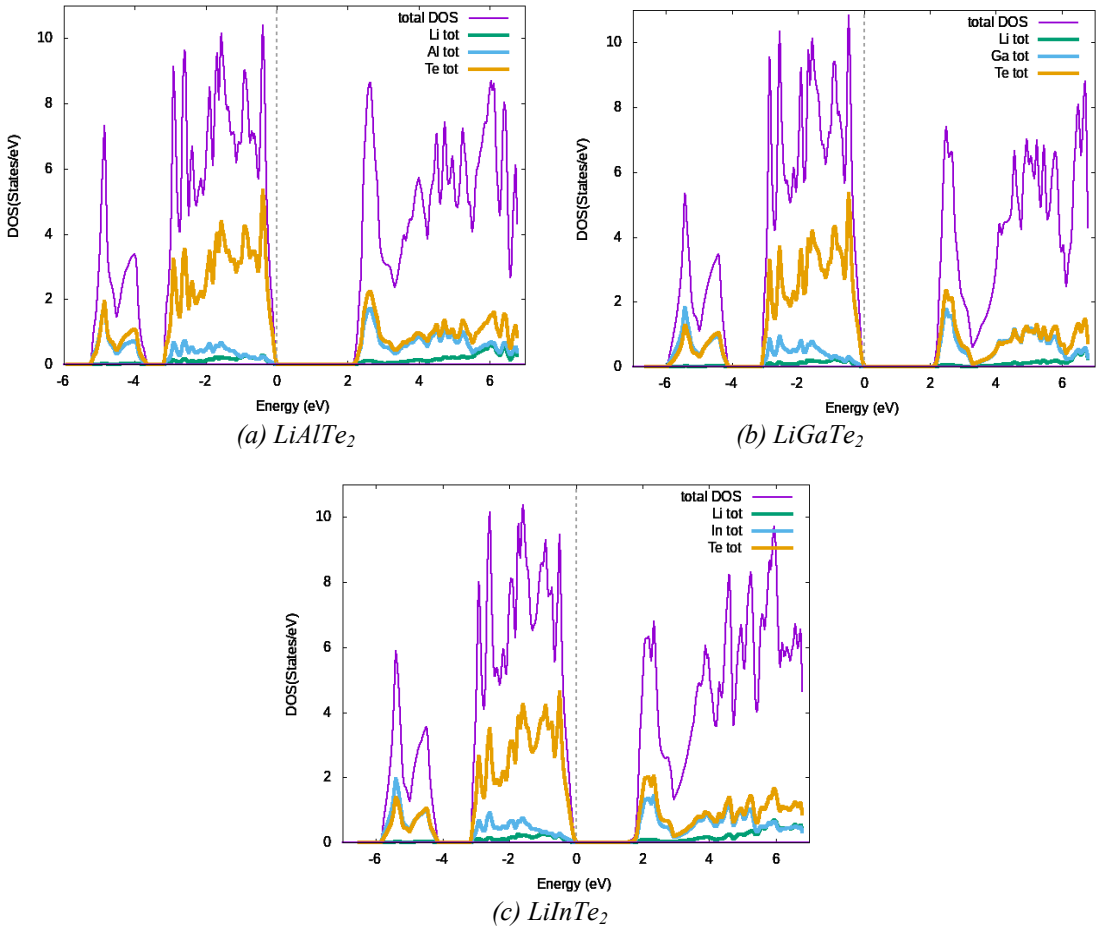
Compounds	**Band-Gap (in *eV*)**				
	LDA	**WC**	**PBE**	**PBEsol**	**Experimental**
$LiAlTe_2$	2.195	2.225	2.290	2.231	2.14 [(a)]
$LiGaTe_2$	1.454	1.487	1.564	1.506	2.31 [(b, c)]
$LiInTe_2$	1.532	1.609	1.719	1.629	1.50 [(d)]

[(a)]Ref [39], [(b, c)] Ref [36, 40] and [(d)]Ref [37].



(a) $LiAlTe_2$ *(b) $LiGaTe_2$* *(c) $LiInTe_2$*

Fig. 3. Band structure curves for $LiXTe_2$ (X = Al, Ga and In) compounds.



(a) $LiAlTe_2$ *(b) $LiGaTe_2$*

(c) $LiInTe_2$

Fig. 4. Total density of states for $LiXTe_2$ (X = Al, Ga and In) compounds.

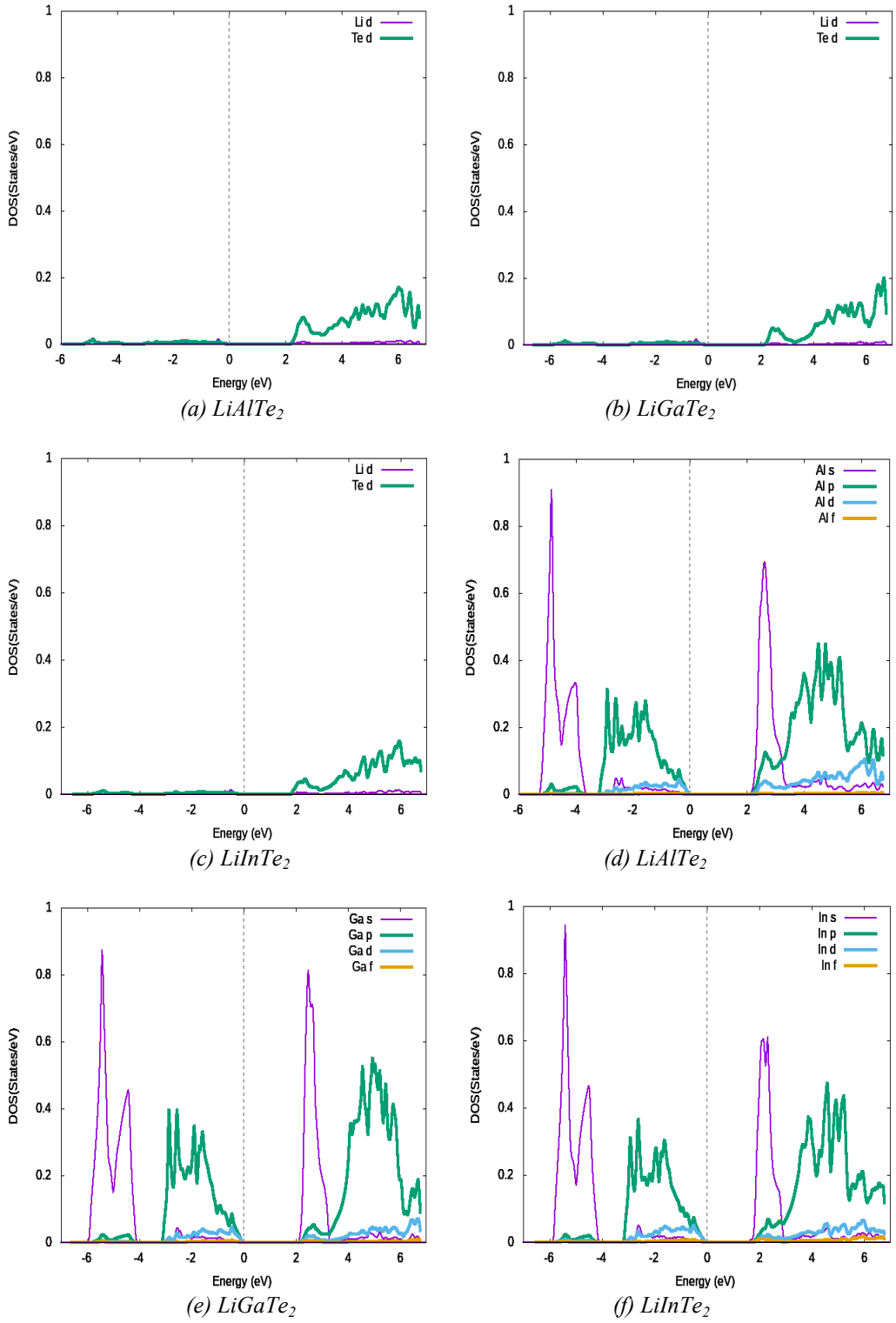


Fig. 4.1. The partial density of states for $LiXTe_2$ (X = Al, Ga and In) compounds. Figure 4.1. (a, b and c) represents the contribution of atoms of the mentioned compounds in d-state and Figure 4.1. (d, e and f) represents the contribution of atoms of the mentioned compounds in s, p, d and f-states.

3.3. Optical Properties

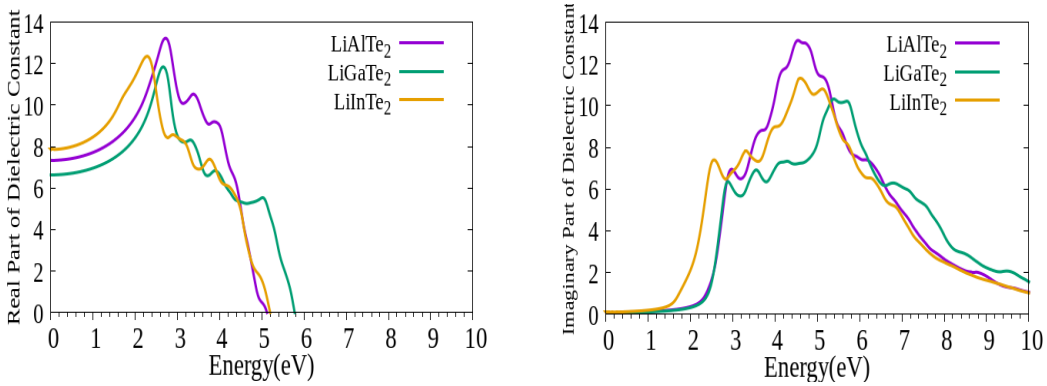
In the solid-state physics, there is lots of importance of the study of various forms of the interaction of light along with matter. The study of optical parameters is the important feature for gaining the proper knowledge of electronic properties of the matters. In manufacturing of optical

instruments, it is very important to investigate the optical parameters of a compound to decide it can be the potential material or not for this purpose. So, for this purpose we have investigated the optical parameters of $LiXTe_2$ (X = Al, Ga and In) chalcopyrite compounds i.e., absorption coefficient, optical conductivity, optical reflectivity, refractive index, extinction coefficient, real and imaginary part of dielectric function and energy loss. The complex dielectric function describes the optical response of matter when the electromagnetic wave incident on the material.

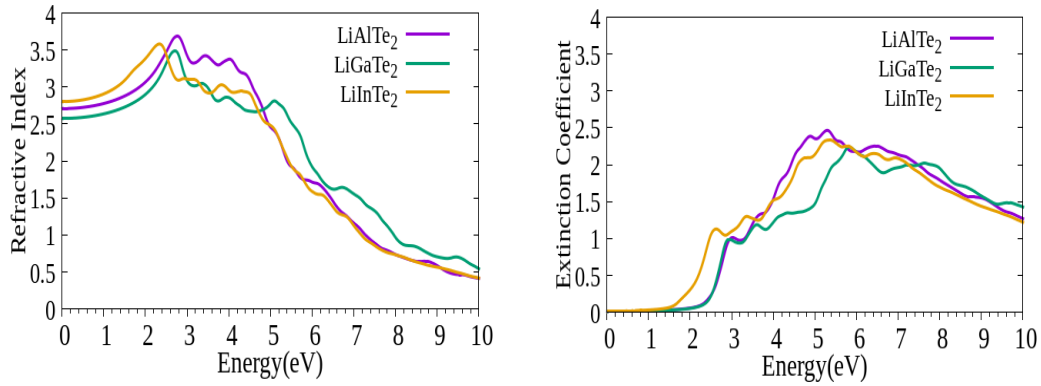
The complex dielectric function is as follows:

$$\varepsilon(\omega)=\varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (1)$$

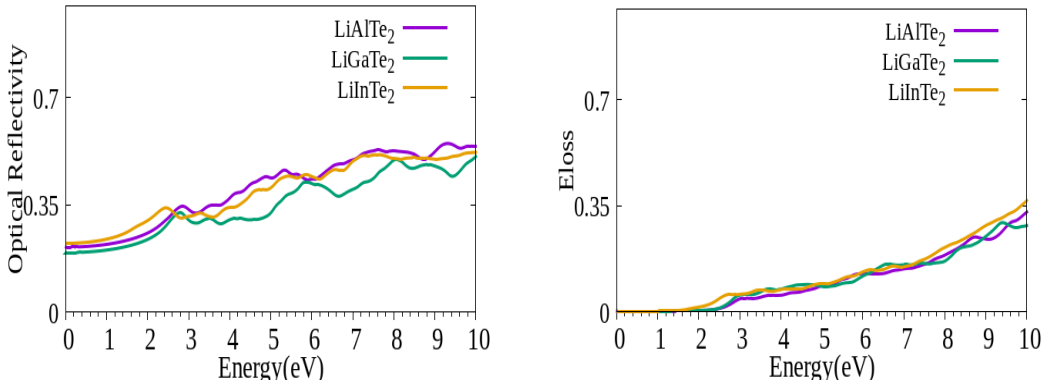
$\varepsilon_1(\omega)$ real part shown the polarization of the compounds when employed the electric field, $\varepsilon_2(\omega)$ imaginary part shown the loss of energy (absorption) in the medium. For understanding the optical spectrum, it is taken into consideration that the transformation phenomena take place from occupied to the unoccupied bands. For investigating the optical properties of the mentioned compounds, the inter band region have been chosen. Calculated optical parameters are shown in the Figure 5 (a-d). From this calculation we noticed that these semiconductors $LiAlTe_2$, $LiGaTe_2$ and $LiInTe_2$ behave very common. From the transformation of electrons from the top of the valence band to the bottom of the conduction band, we got the major peaks in the real part of the dielectric function and in this study these peaks are observe at 2.4 eV for $LiAlTe_2$, 2.2 eV for $LiGaTe_2$ and 2 eV for $LiInTe_2$ further this spectrum starts decreasing up to 3.2 eV for $LiAlTe_2$, 3.3 eV for $LiGaTe_2$ and 2.9 eV for $LiInTe_2$. In the imaginary part of dielectric function, the critical points observed at 1.3 eV for both the compounds $LiAlTe_2$ and $LiInTe_2$ and 2.2 eV for $LiGaTe_2$; we can say that these points are very close to the calculated electronic band gap, so this confirms the accuracy of electronic band gap and this point also called the threshold energy value and from this, we can say that the absorption take place in the UV-region. The dielectric constant at '0' frequency $\varepsilon_1(0)$for $LiAlTe_2$ is 7.31, 6.32 for $LiGaTe_2$ and 8 for $LiInTe_2$ respectively. In Figure 5 (b) the refractive index and the extinction coefficient have shown, we observe that the refractive index for all three compounds increases with the energy approaches high in the visible and UV-region, the major peak for $LiAlTe_2$ is 3.58 at 3 eV, $LiGaTe_2$3.5 is at 2.89 eV, $LiInTe_2$ is 3.56 at 2.21 eV. The refractive index at '0' frequency n (0) for $LiAlTe_2$ is 2.7, 2.58 for $LiGaTe_2$ and 2.8 for $LiInTe_2$. In the spectrum of extinction coefficient k (ω) it is decreasing when photon energy increases for all three semiconductors. In Figure 5 (c) optical reflectivity R (ω) and the electron energy loss $E_{loss}(\omega)$ spectrum have shown, the reflectivity for the mentioned compounds takes in UV-VIS-region and the energy loss is in the IR region of the optical spectrum. In Figure 5 (d) the absorption coefficient $\alpha(\omega)$ and the optical conductivity $\left(\sigma(\omega)\right)$ spectrum has shown, the absorption coefficient measures the value of absorption of photon in a medium of matters. The absorption edges for $LiAlTe_2$ and $LiGaTe_2$ is 2.1 eV and for $LiInTe_2$ is 1.8 eV, and the maximum absorption take place in the UV-region for the mentioned semiconductors. By optical conductivity, we can find the value of the conduction of electron, when electric and magnetic field is applied. From the graphical representation of optical conductivity, we observe that the conductivity of all compounds lies in the UV- region of the EM-spectrum of photons and the major peaks for $LiAlTe_2$ is at 4.98 eV, 6.98 for $LiGaTe_2$ and 5.13 for $LiInTe_2$. From these results of optical parameters, we can say that all three tetragonal (Phase) chalcopyrite semiconductors are suitable compounds for the application of solar cells or photovoltaic cells.



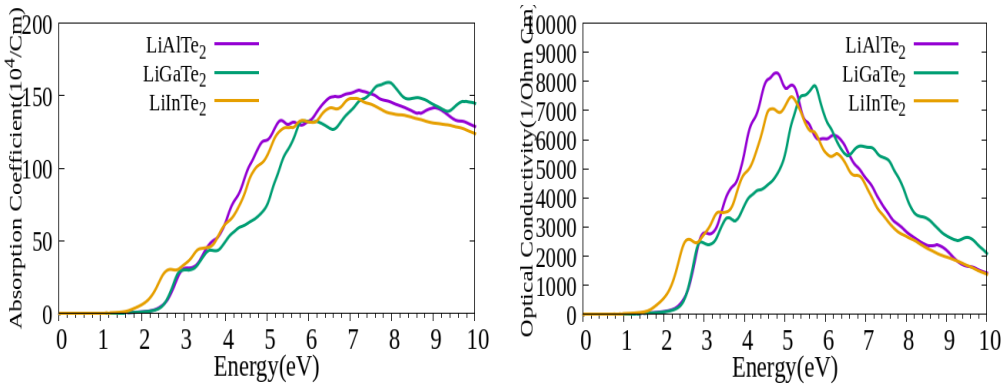
(a) Real and Imaginary part of Dielectric Constants $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ of the mentioned compounds.



(b) Refractive index $n(\omega)$ and Extinction Coefficient $k(\omega)$ of the mentioned compounds.



(c) Reflectivity $R(\omega)$ and Energy loss $E_{loss}(\omega)$ of the mentioned compounds.



(d) Absorption Coefficient $\alpha(\omega)$ and Optical Conductivity $\sigma(\omega)$ of the mentioned compounds.

Fig. 5. The optical parameters of $LiXTe_2$ (X = Al, Ga and In) compounds.

4. Conclusions

In this work, we have been calculated the structural, electronic and optical properties of the $LiAlTe_2$, $LiGaTe_2$ and $LiInTe_2$ chalcopyrite semiconductors by using the WIEN2K simulation package based on the density functional theory. From this study, we have concluded that these compounds possess tetragonal phase structure, direct electronic band gap, which are beneficial for their use in the photovoltaic devices. In the optical spectrum absorption takes place in the UV-region of EM-spectrum. Electron energy loss takes place in the IR-region.

Study of dielectric constant confirms the accuracy of calculated electronic band gaps. The dielectric constant at '0' frequency $\varepsilon_1(0)$ for $LiAlTe_2$ is 7.31, 6.32 for $LiGaTe_2$ and 8 for $LiInTe_2$ respectively and the refractive index at '0' frequency n (0) for $LiAlTe_2$ is 2.7, 2.58 for $LiGaTe_2$ and 2.8 for $LiInTe_2$ respectively. From the study of optical properties, it ensures that all these chalcopyrite compounds $LiXTe_2$ (X = Al, Ga and In) are potential candidates for applications in the photovoltaic devices.

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