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Tuned optoelectronic and thermoelectric properties of $TlMX_2$ through M=Ga,In X=S,Se,Te intercalation

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We presents our analysis on structural electronic and optical properties of TlX and $TlMX_2$ (M =In, Ga; X = Te, Se, S) compound, by first principle density functional theory (DFT).These chalcogenide have a place with a group of the low-dimensionals semiconductors having chains or layered design. They are of critical interested as a result of, their exceptionally anisotropics properties, semiconductivity and photoconductivity, non direct impacts in their IV qualities (counting a district of negatived differentials opposition), exchanging and memories impacts, secondly symphonious opticals age, relaxors conduct and possible application for optoelectronics devices. We reviews the crystals structured of $TlMX_2$ compound, their transports properties below surrounding condition, test and hypothetical investigations of the electronics construction, transports properties and semiconductors metal phased transition below highly tension, and successions of temperature instigated primary phased transition with middle disproportionate state. Electronics natured of the ferroelectrics phased transition in the previously mentione mixes, just as arelaxors conduct, nano domain and conceivable event of quantums specks in dopeds and illuminated precious crystals are examined.

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1. Introduction

Layer structures are observed in WTe2, MoTe2, WSe2, MoSe2, WS2 and MoS2 i.e. group 4-7(Mg). On the other hand, some transitional metals have x for Te, Se, S in case of type MX2. However, the structures MX2 (non-layered) having different kind of structure are occurred in group 8 transition metals. Materials of these kinds have metal atoms possessing a network that is 3D in nature. Also, two approximately similar structures exist; One of them includes Ru, Cu, Fe, Co, Ni, Mn, Os as disulfides regarding pyrite [1,2]. Two types of elements i.e. metals or metalloids are considered as ternary chalcogenide found as a large group of materials. The compounds having x for Te, Se, S while A, B for metallic cations are ternary chalcogenide (AB2X4) possessing special properties along with vital applications are included in this classification. The other structures investigated include M for Fe, Co, Cu i.e. MxRh3-Xs4 (thiorhodites) [3], M for Co, Cu i.e. MCo2S4 (thiocobaltites) , M for Cu, Hg, Zn, Co, Fe, Cd, Ba i.e. MCr2X4 (chalcochromites), M for Cr, Zn, i.e. Mal2S4 (thioaluminates), X for Te, Se, S and A, B for metal cations i.e. AB2X4 (chalcogenide spinels) etc. Also, the ferrimagnetism and ferromagnetism [4], photo magnetic effects [5], thermal conduction in lattice i.e. optical and magnetic properties, semi conductive behavior is observed in spinels of metal chalcogenides. The typical system of valency combination is used to characterize the chalcogenide compounds that are quaternary and ternary in nature.

Insulating behavior is mostly shown by the quaternary chalcogenide because free electrons are absent. The most significant and vital semi conducting and conducting characteristics are

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exhibited by a few chalcogenide materials that are quaternary in nature. A developing area is super conductivity at higher temperature (Tc) related to quaternary chalcogenide. Super conduction at high Tc is obtained by FeSe of rare-earth and alkaline-earth elements, ammonia doping those results in higher temperature superconductivity taken over by compounds of chalcogenide [6]. Information regarding electronic and optical properties of a material is very necessary if we are interested in the utilization of optoelectronic and photonic devices. Materials devices can be known more deeply if these properties are properly studied. Metallic chalcogenide are termed basic materials for conversion of thermoelectric energy, non linear optics, conversion of solar energy, optoelectronics and electronics applications [7]. Having a better agreement with values from experiments, characteristics of quaternary chalcogenide [8] regarding optoelectronics have been investigated successfully with the help of ab-initio calculations.

Researchers are very interested in materials like ternary chalcogenide due to their role in electro optic, non linear optical and optoelectronic devices. Tunable filters and ultraviolet (uv) photo detectors are the applications of CdGa2Se4 and CdAl2Se4 (ternary chalcogenide). Solar cells optimization efficiency is regarded as the basic element that makes these compounds technologically significant. We take X for Se, S, M for Ta, Na, V, Mo, A for Ge, Ga i.e. AM4X8 written for ternary chalcogenide.During a few decades, more interest is taken in nonmetallic and metallic states for investigating their physical properties [9,10].

In this regard, our interest in some $TlMX_2$ (M =In, Ga; X = Te, Se, S) has grown, owing to a scarcity of data on electronic, optical and thermoelectric properties. As a result, we used DFT inside the modified becke johnson potential as implemented in the WIEN2K algorithm to examine the electronic, optical and thermoelectric properties of certain $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds.

2. Computational details and structure description

First of all we have minimized the forces that act on the atoms. By this optimized geometry, we find out the theoretical study of structural electronic and optical properties of TlX and $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds. We studied all these properties by using, full potential linearized augmented plane wave (FPLAPW) through WIEN-2k code [11-18], within the framework of the DFT [19-26]. The exchange correlation energy was calculated by means of the local density approximation (LDA) and the generalized gradient approximation (GGA) [27-38]. At the interstitial region the convergence of energy Eigen values are obtained by expending the wave function, in plane wave basis sets with a cut-off of RMT Kmax=7, where RMT and Kmax, are the smallest muffin-tin radius and largest magnitude of vector K in plane wave expansion, respectively. In order to estimate the physical properties (electronic, structural and optical) of TlX and $TlMX_2$ (M =In, Ga; X = Te, Se, S) compound using the GGA+U formalism. The crystal structure of TlX and $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds have been studied is shown in Fig. 1.

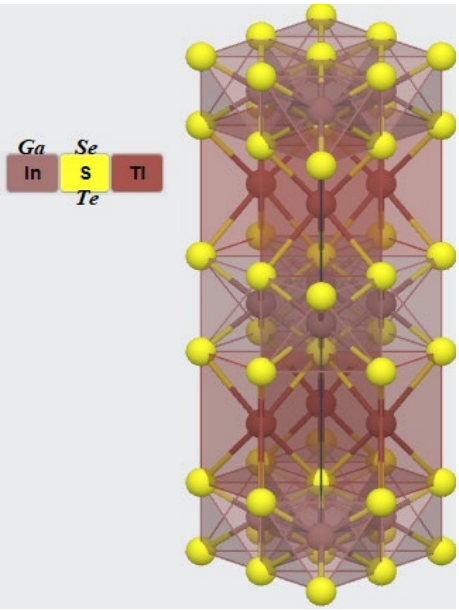


Fig.1. Crystal structure TlX and $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds.

3. Results and discussions

3.1. Electronic properties

3.1.1. Electronic Band structure

The most physical properties of solid materials are related to the electronic band structure; therefore the investigation of electronic band structure is very important. All the optical and charge transport properties of semiconductors are related to the energy band gape and its size. The electronic band structure is investigated with high symmetrical direction in the first Brillion zone (BZ). In this case the highly symmetric points are critical points correlated with unit primitive cell of reciprocal lattice. The coordinates of highly symmetric points depends upon the crystalline structure of the specific symmetry group. For both the real and reciprocal lattices, the unit primitive cell and all the unit vector coefficients are defined by the lattice parameters. The electronic band structure features of investigated TlX and $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds are shown in Figure. 2. We found that by replacing S by Se and Te, band Gap reduces. And also found that the nature changes from indirect to direct nature.

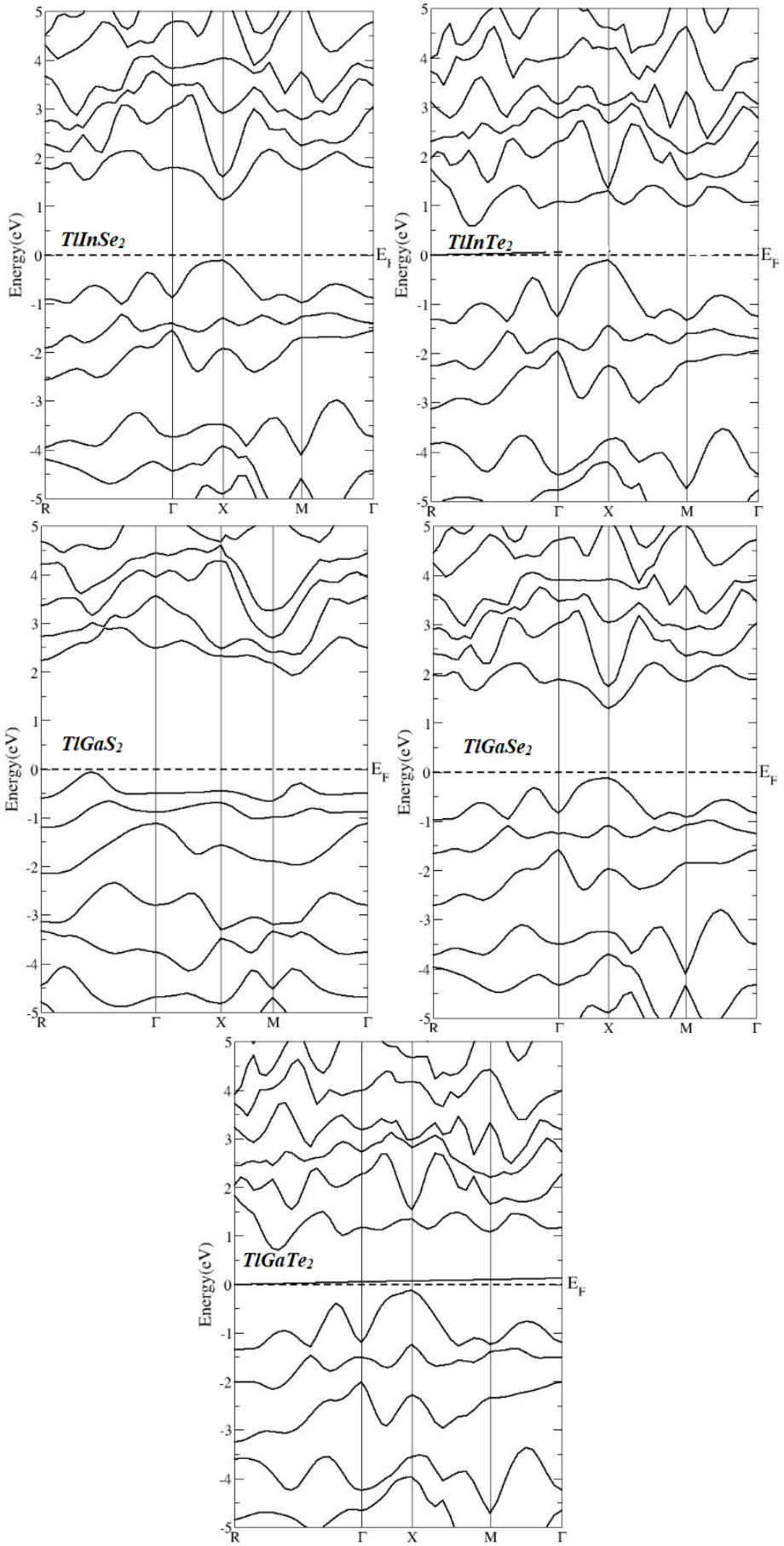
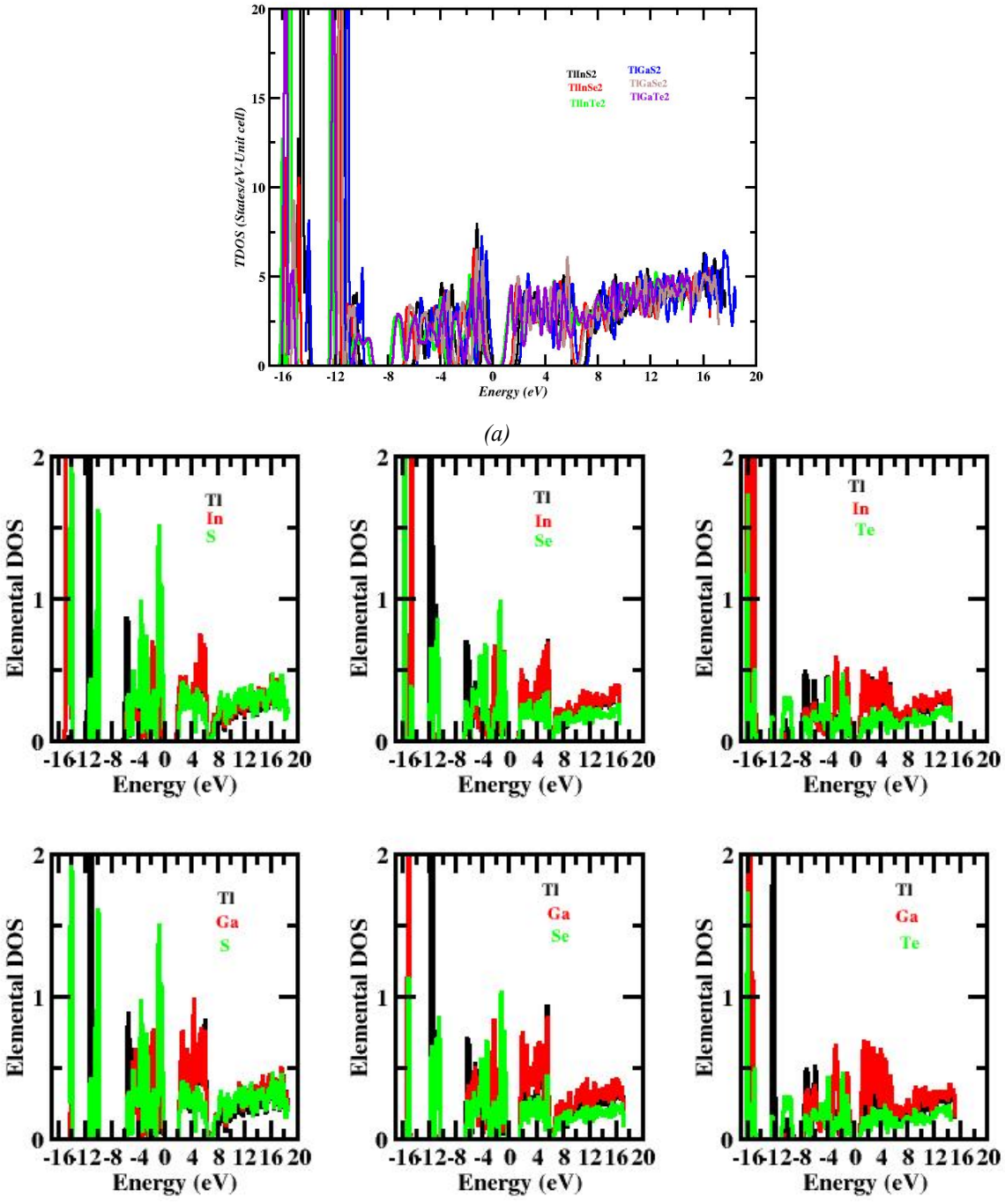


Fig.2. Electronic band structure diagram of $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds.

3.2. Electronic density of states

The investigation of electronic density of state of a compound is to understand the basic features of band structure and the contribution of each atom orbital's to the electronic density of states. The total density of states (TDOS) and partial density of states (PDOS) is linked to the BS, are shown in Figs.3a.Figure 3a represents the electronic density of states of $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds. The TDOS structure show a well defined and broaden energy regions from -17.0 eV to 20.0eV. Here zero energy represents Fermi level (EF). For the total partial density of states (PDOS) for $TlMX_2$ (M =In, Ga; X = Te, Se, S)compound it is observed that the main contribution in the valance band maximum and conduction band comes from the In/Ga and S/Se/Te atoms while the valence band minimum comes from the Tl atom.



(a)

(b)

Fig. 3. (a) Total and (4b)Partial density of states for $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds.

4. Optical dispersion properties

The optical dispersion parameters of energy are mostly due to the electronic band structure. The Investigation of optical properties provides some important basic information. It gives formation regarding filled and unfilled electronic states within the energy band [20]. The optical dispersion properties are very important in the field of optoelectronic device applications. The real $\varepsilon_1(\omega)$ and the imaginary $\varepsilon_2(\omega)$ dispersion parts of the dielectric function are responsible to calculate the important optical properties such as extinction coefficient K(ω), refractive index n(ω), reflectivity R(ω), absorption coefficient I(ω), energy loss function L(ω),and real optical conductivity $\sigma(\omega)$. In this section we will discuss all the optical dispersion properties of $TlMX_2$ (M =In, Ga; X = Te, Se, S compounds.

4.1. Dielectric function dispersion

Fig.4. shows the investigated real and imaginary part of the dielectric constant. For both the compounds $TlMX_2$ (M =In, Ga; X = Te, Se, S), the real part of the dielectric function $\varepsilon_1(\omega)$ and imaginary part $\varepsilon_2(\omega)$ has been shown in Fig. 4a and 4b respectively. The real part $\varepsilon_1(\omega)$ of the dielectric constant is related to the crystal polarizability, which shows direct response of the material with electromagnetic radiations. The values of the real part of dielectric function DF are also directly related to the inter-band dipole probability of transition. Under the limitation of the existence selection rule for the electronic transitions, the dielectric function DF gives the features of the combined density of states DOS near to the Fermi level and the corresponding part of the electronic band structure. From the calculations it is observed that, the peak value of real part of dielectric function$\varepsilon_1(\omega)$ for $TlMX_2$ (M =In, Ga; X = Te, Se, S), as shown in Fig.4a. Our results shows that the value of $\varepsilon_1(\omega)$ remains almost constant (2.25) and (1.5) for both the compounds $TlMX_2$ (M =In, Ga; X = Te, Se, S) from 0eV to 3.0eV, and show a slightly increasing trend up to 5.0eV $TlMX_2$ (M =In, Ga; X = Te, Se, S), beyond this energy, the values of real part of dielectric function$\varepsilon_1(\omega)$ almost remain same up to 8.5eV and 9.5eV for both the compound respectively, further increasing energy correspond again a well defined sharp peak at 9.0eV is observed, behind this energy the value of real part of dielectric function decrease with small fluctuating peaks for both the compounds. After 13.0eV energy, the values of real part of dielectric function $\varepsilon_1(\omega)$ become negative for both the compounds. From investigation it is observed that the values of $\varepsilon_1(\omega)$ shows similar trend for all the compounds.

The imaginary part $\varepsilon_2(\omega)$ (see Fig.4b) of the complex dielectric function (DF) is directly related to the energy band structure of the compound. Here in our calculations the Broadening has been assumed to be 0.1eV which is normally for the smearing due to the electron-phonon interactions. The peaks values for $\varepsilon_2(\omega)$ are almost located at 10.0eV for both the compounds. The values of $\varepsilon_2(\omega)$ are related with the inter-band transition of the same momentum, and intensity depends upon the overlapping of the initial and final states. As per selection rules the optical transitions are permitted only from s-p, p-d and d-p orbitals. The imaginary part $\varepsilon_2(\omega)$ has zero values up to the 4.5eV for all the compounds, the further increase in energy 10.0eV, the imaginary part $\varepsilon_2(\omega)$ show a slow increase with small fluctuating peaks for all the compounds. From the investigation it is has been observed that the overall spectral behaviour for the imaginary part of dielectric function $\varepsilon_2(\omega)$ is similar for all.

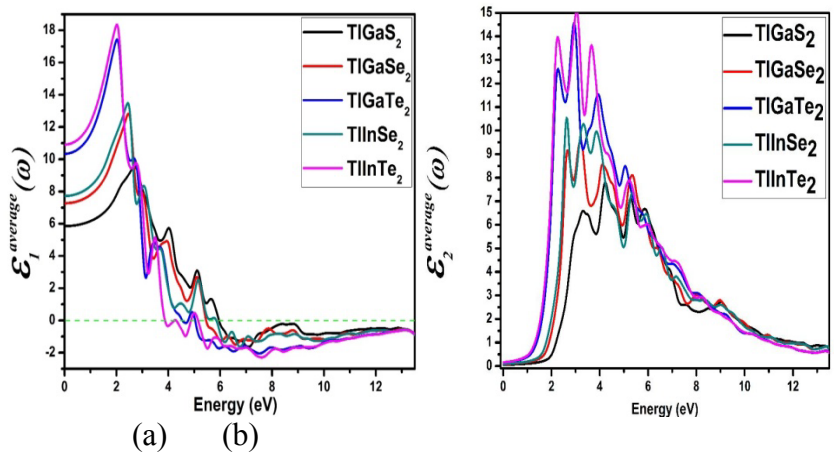


Fig.4. (a): Real part $\varepsilon_1(\omega)$ and (b): Imaginary part $\varepsilon_2(\omega)$ of complex dielectric function of $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds.

4.2. Energy Loss function L(ω)

The energy-loss function $L(\omega)$ is related to the energy loss of very fast moving electrons crossing the material, it is a very important optical parameter and also related to the imaginary part of complex dielectric function. Figure 5 shows the energy loss function $L(\omega)$ against energy. The peaks in energy loss function $L(\omega)$, are due to a specific behavior called plasma oscillations, and the related frequencies are so-called plasma frequencies. The dominant peaks for $L(\omega)$spectra arise, due to the Plasmon excitations. The resion behind this is the collective longitudinal response of valance electron oscillations against the background atomic cores with plasma frequency Electronic mobility behavior in a materials and associate energy with them can be explain by the behavior of average energy loss function. Electronic mobility can be explained that how fastly electron move in a mediumand semiconductor when pull by an electric field. In the given figure energy loss started from 2 e V and small changes occur in energy level to about nearly 4 e V. At the end the sharped peaks appeared at 13 e V. The given figure shows that energy loss functions behave an isotropic behavior.

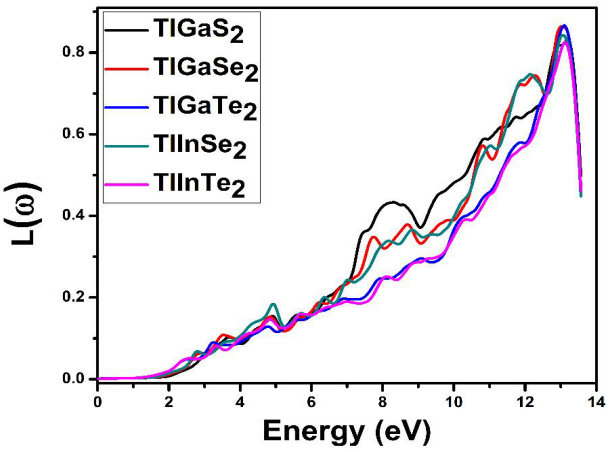


Fig.5. Energy loss function $L(\omega)$ of $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds.

4.4. The refractive index n(ω)

The refractive index n(ω)of a material is simply the ratio of the speed of light in free space to the speed of light in a given material. Fig.6. show the refractive index variation against spectral energy for $TlMX_2$ (M =In, Ga; X = Te, Se, S) compoundscompounds. The average of five non zero components of the optical refraction n(ω) exhibits that there is no such evident change in refraction spectrum with respect to different material concentrations in $TlMX_2$ compound and it is also obvious from the Fig.6. A remarkable increase in refraction value is observed with small fluctuating peaks and they are associated with inter-band transitions.The sudden increase in refraction after 2 eV and approaches 4eV and then decrease, as can be seen from the Fig.6 Our investigated compounds also exhibit good refraction value at higher energy range (5-7 eV). It is worthy to emphasize that all the five compounds have shown a good refraction value both in the visible and ultraviolet region of spectrum.

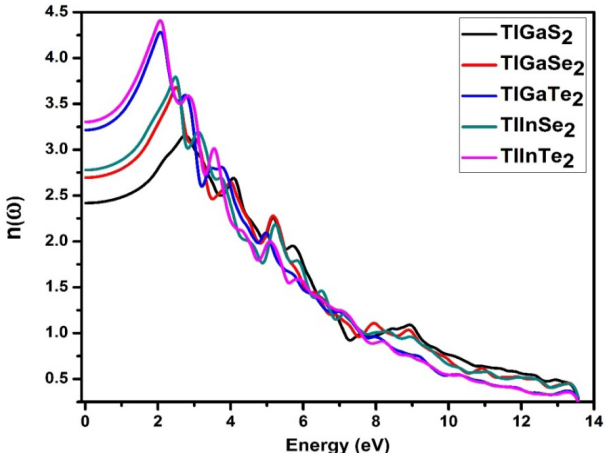


Fig.6. Refractive index $n(\omega)$ of $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds.

4.5. The Reflectivity R(ω)

The reflectivity dispersion R(ω) is related to the reflection of electromagnetic radiations from the material. Figure 7 shows the reflectivity R(ω) of $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds, against spectral energy, The average of five nonzero components of the optical reflectivity coefficient $R^{avg}(\omega)$exhibits that there is no such evident change in reflectivity spectrum with respect to differentmaterial concentrations in $TlMX_2$ compound and it is also obvious from the Fig.3. A remarkable increase in reflectivity value is observed with small fluctuating peaks and they are associated with inter-band transitions.The sudden decrease in reflectivity at 8.5eV and approaches 9Ev and the nincreases, as can be seen from the Fig.8 Our investigated compounds also exhibit good reflectivity value at higher energy range (10-12 eV). It is worthy to emphasize that all the five compounds have shown a good reflectivity value both in the visible and ultraviolet region of spectrum.

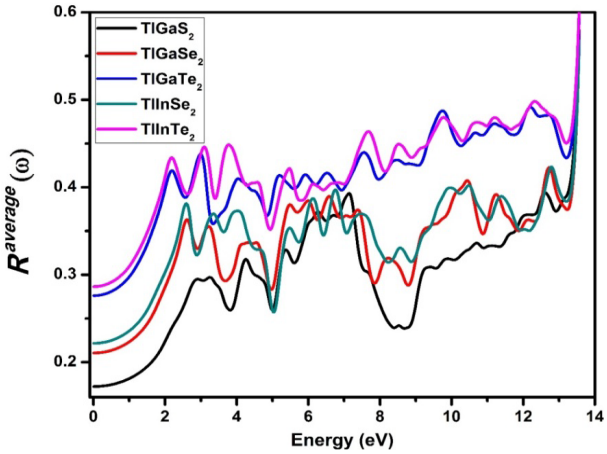


Fig.7. Reflectivity $R(\omega)$ *of* $TlMX_2$ *(M =In, Ga; X = Te, Se, S) compounds.*

4.6. Absorption coefficient I(ω)

Absorption coefficient I(ω) is concerned with the penetration of an electromagnetic wave of fixed energy through a material, it means that, how much deeply an electromagnetic wave penetrate in a specific material before absorption. The absorption spectra I(ω) formed due to the different inter-band transitions The arrived at the midpoint of qualities for each of the five component of absorption coefficient are plotted in Fig.8. The spectra for all the examined compound show practically comparative pattern, however show a slight variety from one another with critical anisotropy. The absorption threshold energy related to their band gaps was found at energies about 2 eV for each compound. Besides, the determined absorption coefficient range has demonstrated a most extreme at 6eV to 10eV for all the examined compound. The bend is diminished till 13eV and afterward the range increase till 14 eV. An ideal material for the photovoltaic applications generally displays direct band hole that could fascinate in the fundamental piece of the obvious light range with little reflectance and huge absorption coefficient. As indicated by our computed outcomes the $TlMX_2$ compounds uncovered that they can be utilized for the photovoltaic applications.

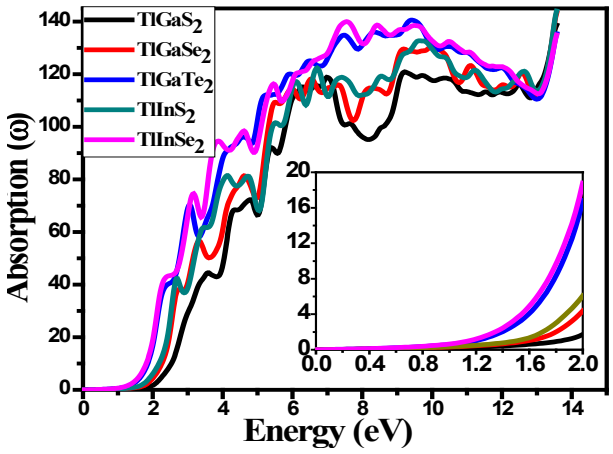


Fig.8. Absorption coefficient I(ω) of $TlMX_2$ *(M =In, Ga; X = Te, Se, S) compounds.*

4.7. Real optical conductivity $\sigma(\omega)$

The real optical conductivity $\sigma(\omega)$ is related to the electrical conductivity in the presence of electromagnetic radiations. The word "optical" here covers the whole frequency range, and is not limited only to the visible region of the electromagnetic spectra. Electrical conductivity is very close to electrical conductance. The figure.9 show that at point 2 e V electrical conductivity decreases due to various behavior of particular charge concentration, and maximum electron conductivity at point 6 e V.

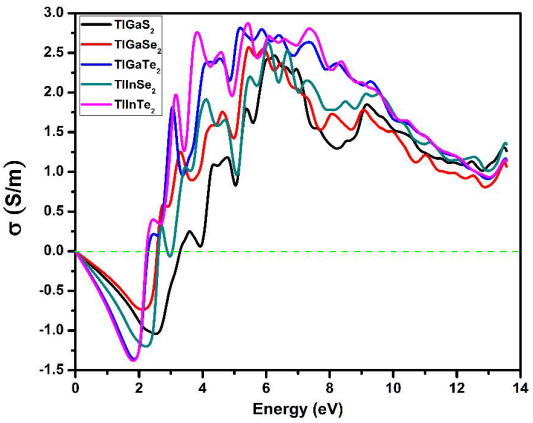


Fig.9. Real optical conductivity $\sigma(\omega)$ of $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds.

4.7. Electrical conductivity (σ)

The electrical transport properties directly influenced by the energy band structure of the material. We have explored the thermoelectric properties of $TlMX_2$, M=Ga,In X=S,Se,Te, as shown below. The calculated electrical conductivity (σ) for investigated compounds shows different behavior due to the particular charge concentration. The electrical conductivity plots under constant relaxation time *vs* temperature (T) are depicted in Fig.6. The electrical conductivity increases with increase in temperature for $TlGaS_2$, $TlGaSe_2$, $TlGaTe_2$ and $TlInTe_2$this is due to the increase in concentration of electrons. While for the $TlInS_2$ and $TlInSe_2$ decreases with increase in temperature this is due to the increase in concentration of hole. The concentration of carriers (Electron/hole) and their mobility increases almost with temperature. These compounds pretends to be a typical n/p-type semiconducting nature and there calculated conductivity is mainly induced by the electron carrier concentrations.

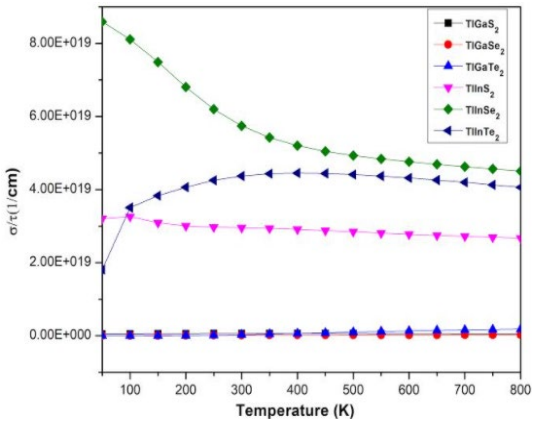


Fig. 10. Electrical conductivity $\sigma(\omega)$ of $TlMX_2$ (M =In, Ga; X = Te, Se, S) compounds.

5. Conclusions

In this study we investigate the structural, electronic, and optical properties of the chalcogenides compound $TlMX_2$ compounds. It is an important group of the chalcogenides compound $TlMX_2$containings $TlGaS_2$, $TlGaTe_2$, and $TlInSe_2$ were studying by using computational method, density function theory (DFT), in light of the primary standards. The determined primary information is as per the accessible exploratory outcomes. The noticeable progress tops in the genuine and fanciful pieces of the dielectrics work and opticals constant (refraction record, reflectivities and optical conductivity) changed by supplanting X to the components S, Te, and Se_2. The energies of the pinnacles changed in a diminishing mannera X is supplanted by Se_2, S, and Te in provided request. The highly absorptions and reflectivities tops show the utilities of these compound in optoelectronics devices. The temperature reliance of some significant properties, for example, the Seebecks coefficients, the electrical conductivities, the warm conductivities, and the figures of value of that compound demonstrate that can be considered as reasonable possibility for significant application in the field of thermo-electric energy.

To summarize, we expect that the study will motivate researchers to investigate the interesting properties of chalcogenides $TlMX_2$ compounds in more detail, both theoretically and experimentally in future.

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