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Anion-Cation Replacement Effect on the Structural and Optoelectronic Properties of the LiMX₂ (M = Al, Ga, In; X = S, Se, Te) Compounds: A First Principles Study

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Abstract: In the chalcopyrite (or tetragonal) phase, different physical properties of the ternary LiMX₂ (M = Al, Ga, In and X = S, Se, Te) compounds are studied by the very accurate density functional method. The optimized lattice constants and the bandgaps are close to the existing experimental data. In addition, for most of the LiMX₂ compounds, when the cations change from Al to In and anions from S to Te, the lattice constant and equilibrium volume for the crystal unit cell increase whereas the bulk modulus decreases. Using different generalized gradient approximations, the band structure calculations are performed. Generally, it was observed that there exists a decreasing tendency of the bandgap energies except for the LiAlSe₂, LinSe₂, and LiGaTe₂ compounds due to the change from Al to In as well as the change from S to Te. The bonding analysis shows that ionic bonds are present between the Li-X atoms, while a covalent bond exists between the M cations and X anions. The optical properties of the compounds are studied by calculating the real and imaginary components of the refractive index, reflectivity, optical conductivity, and birefringence. In addition, the optical properties from the calculations show that these materials are appropriate applicants to be utilized as Bragg’s reflector or applied in optoelectronic and solar cell technology.

Keywords: Chalcopyrites; Electronic Properties; Optical Properties; Structural Properties.

1 Introduction

Ternary chalcopyrite semiconductor materials have become the backbone of modern technology [1, 2] due to their outstanding electrical, structural, and optical properties [3–7]. In recent years, these ternary semiconductors with the general formula A'B'C₂X₂, e.g. LiMX₂ (M = Al, Ga, In and X = S, Se, Te), had received substantial attention owing to their valuable applications in both nonlinear optical and optoelectronic devices [8–11]. These LiMX₂ compounds are also suitable applicants for the solar cells [12], light-emitting diodes [13], and nonlinear optical devices [14] along with optical frequency conversion applications in solid state tunable laser systems [15, 16]. In addition, ternary chalcopyrite LiMX₂ (M = Al, Ga, In and X = S, Se, Te) semiconductor compounds could be developed as thin films that are mostly required for solar panel applications. Most of the LiMX₂ compounds have a bandgap in the infrared [17] to ultraviolet regions [18] in the electromagnetic spectrum, which makes these materials essential for the solar cell technology, especially the LiAlSe₂ and LinSe₂ compounds that have bandgaps in the visible portion of the electromagnetic spectrum [19].

Recently, there is high demand for the detection of radiation for the scientific and security applications, where the standard technology based on He gas exists, but there is a shortage of He gas globally. Hence, chalcopyrite compounds can fulfill this need if the lithium-based LiMX₂ (M = Al, Ga, In; X = S, Se, Te) compounds are properly developed [5]. These are also used in the terahertz devices [20, 21]. Lithium-based LiMX₂ (M = Al, Ga, In and X = S, Se, Te) compounds are experimentally observed to have 122 (I4̅2 d) symmetry group and 42 months point group of the chalcopyrite structure, as represented in Figure 1. It is clearly observed from the figure that the doubly zinc structure forms the chalcopyrite unit structure where the arrangement of the cations is similar while the arrangement of the anions is positioned at different locations in the unit cell [22].

The LiMX₂ (M = Al, Ga, In; X = S, Se, Te) compounds have received high interest from theoretical point of view. Mechanism of the linear and nonlinear photonic effects of chalcopyrites LiGaX₂ (X = S, Se, and Te) compounds were studied by the Bai et al. [9]. Kosobutsky and Basalaev [6] have studied the energy bandgaps, density of states, and different optical parameters of the LiMTe₂ (M = Al, Ga, In) compounds in the chalcopyrite structure. Later on, they [7] have investigated the electronic band profiles
2 Computational Details

The calculations corresponding to the physical properties of the LiMX_2 compounds are performed with the FP-LAPW + lo method as implemented in the WIEN2k code [28]. This is one of the most flourishing computational techniques to study the ground state properties of materials based on the DFT. To treat the exchange correlation potential, the Wu-Cohen generalized gradient approximation [29] and Engel-Vosko GGA (EV-GGA) were used [30]. According to the FP-LAPW + lo method, the division of the unit cell consists of two parts that are inside and outside of the muffin tins (MT). The electron density inside of the MT is denoted as the core electrons, whereas the electron density in the interstitial regions (outside of the MTs) is denoted as the valence electrons. Relativistic approach was applied to handle the core electrons while scalar relativistic approach was applied to treat the valence electrons. Different bases sets were used to expand the wave functions in the two different regions of the unit cell. Inside the MTs, the wave functions in non-overlapping spheres of MT radii (R_MT) are expanded in spherical harmonic up to \( l_{\text{max}} = 10 \). The value of \( R_{MT} \) was selected in such a manner that there are no possibilities for the charges to leak out from the MT sphere and the total energy convergence was achievable. In the interstitial region, the plane wave cut-off for the LiMX_2 (M = Al, Ga, In and S, Se, Te) compounds is chosen at \( K_{\text{max}} \times R_{MT} = 7.0 \) for the wave function expansion. For the chalcopyrite structure, the suitable \( R_{MT} \) values in the range of 2–2.5 Bohr are chosen for the Li, Al, Ga, In, S, Se, and Te atoms. The expansion of the charge density and potential up to \( G_{\text{max}} = 12 \, (\text{Ry})^{1/2} \) in the interstitial region are represented by the Fourier series.

In addition, to obtain better results, the calculations are computed with a mesh of 500 \( k \)-points in the irreducible Brillouin zone (BZ). The self-consistent iterations end when the alteration in the absolute value of the total energy convergence is less than \( 10^{-4} \, \text{Ry} \).

3 Results and Discussion

3.1 Structural Properties

The crystal structure of the ternary semiconductor LiMX_2 compounds is shown in Figure 1. The structural properties of the ternary LiMX_2 semiconductor compounds are calculated by using the Birch Murnaghan’s equation of state [31] in which we fitted the unit cell volume versus total energy. When the compounds have been optimized,
we obtain the ground state minimum equilibrium energy ($E_0$), equilibrium volume ($V_0$), and equilibrium lattice constant ($a_0$ (Å)). In addition, the bulk modulus, $B_0$ (GPa) and its pressure derivative are also calculated from the energy optimization. Figure 2 represents the optimization plot for the LiAlS$_2$ compound in the chalcopyrite phase, respectively, as a prototype for the LiMX$_2$ compounds. The anion-displacement parameter value in the chalcopyrite phase is calculated theoretically by the structure relaxation method, where the theoretically calculated value of internal parameter $u$ obtained by this method is more accurate. From Table 1, it is clear that the lattice constant values increase from the Al to In cations and from the S to Te anions except for the LiAlSe$_2$ and LiGaTe$_2$ compounds. Conversely, the bulk modulus value except for the LiAlSe$_2$ and LiGaS$_2$ compounds decreases when shifting from the Al to In atoms and also similarly reduces when shifting from the S to Te atoms. The derivative of the bulk modulus $B'_0$ value is constant for the various LiMX$_2$ compounds, which is about 5. In addition, the rigidity of a crystal can be indicated from the bulk modulus value, where a larger value of the bulk modulus implies that a crystal is more rigid. The decrease in the bulk modulus value of the LiMX$_2$ compounds is responsible for the high compressibility and reduced hardness in the compounds.

### 3.2 Electronic Properties

The electronic properties of the ternary LiMX$_2$ semiconductor compounds in the chalcopyrite phase are described by the calculation of the electronic band structures as well as the partial and total densities of states in the reduced zone scheme by using the Wu-Cohen GGA and EV-GGA. Using the EV-GGA approximation, the electronic band structures are depicted in Figure 3. The calculations indicate that the bandgap nature of all these LiMX$_2$ compounds are direct except for the LiAlTe$_2$ and LiGaTe$_2$ compounds due to the maxima and minima of the valence and conduction bands, respectively, positioned at the same $\Gamma$ symmetry point of the BZ ($\Gamma$-$\Gamma$). The maxima of the valence bands in the LiAlTe$_2$...
and LiGaTe₂ compounds are situated at Γ symmetry point, and the minima of the conduction bands are situated at the H symmetry point of the BZ; hence, the bandgaps of these compounds are indirect. The computed energy bandgaps together with the experimental and theoretical calculations of the LiMX₂ compounds are tabulated in Table 2. Although our computed bandgap values of the LiMX₂ compounds with the EV-GGA are lesser than the experimental values, they are also in close agreement with the other theoretical calculations, where such an underestimation of the bandgap values are acceptable for the density functional theory based methods. From Table 2 for the LiMX₂ compounds, it is clear that except for the LiAlSe₂, LiInSe₂, and LiGaTe₂ compounds, the bandgap values decrease from the S to Te atoms and also from the Al to In atoms, respectively.

The density of state plots for the LiMX₂ (M = Al, Ga, In and X = S, Se, Te) compounds in the chalcopyrite (tetragonal) phase is shown in Figure 4. The Fermi level has been chosen at 0 eV, and to the left of the Fermi level, the valence band is divided into two regions. In the region with energy from −3 to −6 eV, the hybridization between the Al, Ga, and In s states and the S, Se, and Te p states is responsible for the covalent bonding nature. The closest region to the Fermi level is from 0 to −3 eV; the main contribution in this region comes from the Al, Ga, and In p states and the S, Se, and Te p states as well as smaller contributions from the Li s state. In the conduction band from 0 to 6 eV, the hybridization occurs among the Al, Ga, and In s states and the S, Se, and Te p states as well as some contributions from the Ga and In p states in this region.

In order to comprehend the bonding nature in the LiMX₂ (M = Al, Ga, In and X = S, Se, Te) compounds, the electronic charge density distribution plays an important role, where Figure 5 represents the contour maps of the valence charge density of the compounds in the 2D (110) plane. Charges are easily transferred when the electronegativity difference between the atoms is large, which is responsible for the ionic bonds between the atoms. Conversely, the covalent bond occurs between atoms when the electronegativity difference between atoms is small, hence due to charges sharing covalent bond formed. The electronegativity difference between the Al (1.61) and S (2.58), Al (1.61) and Se (2.55), Al (1.61) and Te (2.1), Ga (1.81) and S (2.58), Ga (1.81) and Se (2.55), Ga (1.81) and Te (2.1), In (1.78) and S (2.58), In (1.78) and Se (2.55), and the In (1.78) and Te (2.1) atoms are 0.94, 0.97, 0.49, 0.74, 0.77, 0.8, and 0.32, respectively, where the values in the parentheses denote the electronegativity of the respective atoms. The values of the electronegativity difference between the M cation and X anion are small, which indicates the sharing of charges; hence, covalent bond forms between the M cation and X anion, respectively. It is also clear from Figure 5 that the sharing of charges between the M cation and X anion raise, which causes the covalent bonding nature. From the electronic charge density, it is clear that the covalent bond forms due to the hybridization of the sp state of the anion and cation. In addition, the covalent bond characters increase from

![Figure 3: Band structures of the LiMX₂ (M = Al, Ga, In and X = S, Se, Te) compounds in the chalcopyrite (tetragonal) phase that are calculated with the EV-GGA potential.](image)

**Table 2:** The computed bandgap values (in eV) of the LiMX₂ (M = Al, Ga, In and X = S, Se, Te) compounds in the chalcopyrite phase as compared with other experimental and theoretical values.

<table>
<thead>
<tr>
<th>Compounds</th>
<th>GGA</th>
<th>EV-GGA</th>
<th>Exp.</th>
<th>Other cal.</th>
</tr>
</thead>
<tbody>
<tr>
<td>LiAlS₂</td>
<td>3.13</td>
<td>4.13</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LiAlSe₂</td>
<td>0.08</td>
<td>0.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LiAlTe₂</td>
<td>1.74</td>
<td>2.13</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LiGaS₂</td>
<td>2.37</td>
<td>3.03</td>
<td>4.15</td>
<td></td>
</tr>
<tr>
<td>LiGaSe₂</td>
<td>1.07</td>
<td>1.62</td>
<td>3.34</td>
<td></td>
</tr>
<tr>
<td>LiGaTe₂</td>
<td>0.94</td>
<td>1.40</td>
<td>2.41</td>
<td>2.3³</td>
</tr>
<tr>
<td>LiInS₂</td>
<td>1.85</td>
<td>2.35</td>
<td>3.59</td>
<td></td>
</tr>
<tr>
<td>LiInSe₂</td>
<td>1.45</td>
<td>2.07</td>
<td>2.86</td>
<td>2.05</td>
</tr>
<tr>
<td>LiInTe₂</td>
<td>1.6</td>
<td>2.15</td>
<td>2.41</td>
<td>1.31, 2.40³</td>
</tr>
</tbody>
</table>

*¹[16], ²[18], ³[33], ⁴[5], and ⁵[35].
the cations Al and Ga to In. The electronegativity difference between the Li and S, Li and Se, and the Li and Te atoms are 1.6, 1.57, and 1.12, respectively, which are large; hence, the bonds between Li and X anions are ionic. Furthermore, the ionic bonds weaken from S to Te; hence, the LiMX$_2$ (M = Al, Ga, In and X = S, Se, Te) show partially ionic and covalent bond characters.

3.3 Optical Properties

Refractive index is an important parameter that is used for the understanding of the optical-related properties and the propagation of light through different materials where absorption and refraction are explained by the single optical quantity known as complex refractive index, which is represented by $\tilde{n}(\omega)$:

$$\tilde{n}(\omega) = n(\omega) + ik(\omega)$$  \(1\)

In (1), $n(\omega)$ is the normal refractive index, which is the real component of the complex refractive index, and $k(\omega)$ is the extinction coefficient of $\tilde{n}(\omega)$, which is also the imaginary component of $\tilde{n}(\omega)$. The $k(\omega)$ coefficient indicates the loss of the energy of a photon when it propagates through a material medium. It has a very significant interpretation in solid state devices such as solar cells, photonic crystal detectors, and wave guides. For the tetragonal crystal system, two tensor components are necessary for the complete interpretation of the material’s optical properties.

Figure 6 represents the frequency-dependent parallel and perpendicular components of the refractive index $[n_{\parallel}(\omega)$ and $n_{\perp}(\omega)]$ as well as the extinction coefficient $[n_{\parallel}(\omega)$ and $n_{\perp}(\omega)]$ of the refractive index (the solid and dotted lines denote the parallel and imaginary components of the refractive index, respectively). The values of $n(0)$, which is the parallel static component of the normal refractive index, and $n_{\perp}(0)$, which is the static perpendicular component of the refractive index, are calculated and depicted in Table 3. Figure 6 indicates that at energies from the zero frequency, the parallel and perpendicular components of $[n_{\parallel}(\omega)$ and $n_{\perp}(\omega)]$ increase, and at certain values of energies, they attain the maximum peak values. With further increase in energy, the magnitude of these $[n_{\parallel}(\omega)$ and $n_{\perp}(\omega)]$ components decreased, and after several oscillations, the magnitude of the $[n_{\parallel}(\omega)$ and $n_{\perp}(\omega)]$ spectra decreases beneath unity. In this region with $n(\omega) < 1$, the
phase velocity is greater than the speed of light. However, the group velocity in this region is always smaller than the speed of light; hence, the relativity relation is not violated. Due to the change of the anions from S to Te and also the change of the cations from Al to In, the peaks of the \( n_{||}(\omega) \) and \( n_{\perp}(\omega) \) spectra shift toward the lower energy that are to be similar to the reduction of the energy bandgaps of the LiMX\(_2\) (M = Al, Ga, In and X = S, Se, Te) compounds except for the LiInSe\(_2\) and LiInTe\(_2\) compounds. In addition, the calculated peak values of the refractive index \( n_{||}(\omega) \) and \( n_{\perp}(\omega) \) along with the static refractive index depend on the frequency. The birefringence (\( \Delta n \)) of the compounds is plotted versus energy as shown in Figure 7 where the birefringence, range of anisotropy, and the maximum value of anisotropy are tabulated in Table 3. The birefringence values corresponding to all the LiMX\(_2\) (M = Al, Ga, In and X = S, Se, Te) compounds are small and negative except for the LiInSe\(_2\) and LiInTe\(_2\) compounds whose values are positive.

Figure 6 also shows the extinction coefficient, \( k(\omega) \), with the parallel and perpendicular \( k_{||}(\omega) \) and \( k_{\perp}(\omega) \) components of the LiMX\(_2\), where 3.3, 0, 2.1, 1.5, 1.0, 0.6, 1.3, 1.1, and 0.6 are the threshold energy of the \( k_{||}(\omega) \) spectra for the LiAlS\(_2\), LiAlSe\(_2\), LiAlTe\(_2\), LiGaS\(_2\), LiGaSe\(_2\), LiGaTe\(_2\), LiInS\(_2\), LiInSe\(_2\), and LiInTe\(_2\) compounds, respectively. Above these energies, the parallel and perpendicular components of the \( k(\omega) \) spectra gradually increase with a few peaks, and at particular energy, the \( k_{||}(\omega) \) and \( k_{\perp}(\omega) \) spectra attain the maximum peak values. At this peak energy, the LiMX\(_2\) compounds show maximum absorption, and with further increases in energy, the magnitudes of the \( k_{||}(\omega) \) and

**Figure 5:** The electronic charge density contours of the LiMX\(_2\) (M = Al, Ga, In and X = S, Se, Te) compounds.
$k(\omega)$ spectra (or absorption) decrease with small oscillations where the various peaks are observed owing to the electronic transition from the occupied valence band to the unoccupied conduction band. Maximum absorption is observed in the energy ranges of 5.00–12.00, 0.5–9.2, 3.4–11, 4.3–12, 2.3–12, 2.1–11.2, 3.8–12, 3–12, and 3–11.6 eV for the LiAlS$_2$, LiAlSe$_2$, LiAlTe$_2$, LiGaS$_2$, LiGaSe$_2$, LiGaTe$_2$, LiInS$_2$, LiInSe$_2$, and LiInTe$_2$ compounds, respectively. Anisotropy is observed in the energy ranges from 0 to 12 eV, and beyond these energy ranges, the parallel and perpendicular components of the $k(\omega)$ spectra (absorption coefficients) become isotropic. The anisotropic peak values of $k(\omega)$ are negative for most of the compounds except for the LiInSe$_2$ compound, which can be observed from Figure 7. In addition, the absorption peaks shift toward the lower energies with the change from the S to Te anions in the LiMX$_2$ compounds. Important data corresponding to the extinction coefficients that are related to the LiMX$_2$ compounds are calculated and listed in Table 3. Maximum absorption peaks are noticeable in both the visible and ultraviolet parts of the electromagnetic spectra; therefore, these materials are ideal for solar cell applications. The static refractive index value is greater than 2, which indicates that these compounds have useful application in photonic devices.

The frequency-reliant reflectivity, $R(\omega)$, of the LiMX$_2$ compounds with the electric field polarization that is parallel and perpendicular to the c-axis [$R_\parallel(\omega)$ and $R_\perp(\omega)$] are plotted in Figure 8. The static reflectivity at the zero frequency for the parallel and perpendicular components of the reflectivity spectra is denoted as $[R(0), R_\perp(0)]$, respectively. Moreover, above the zero frequency, the reflectivity spectra of the LiMX$_2$ compounds increase and attain maximum value after several oscillations and then start to decrease to lower magnitude at higher energies. Except for the LiAlSe$_2$ compound, the peaks of the $R(\omega)$ spectra

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**Figure 6:** The real component, $n(\omega)$, and the imaginary component, $k(\omega)$, of the refractive index of the LiMX$_2$ (M = Al, Ga, In and X = S, Se, Te) compounds through the EV-GGA potential.
Table 3: The computed static refractive indices \( n(0) \) and \( n'(0) \), birefringence \( \Delta n(0) \), maximum \( n(\omega) \) and \( n'(\omega) \) values, energy values at \( n(\omega) < 1 \) and \( n'(\omega) < 1 \), anisotropy range for the refractive indices, absorption edge values for \( k(\omega) \) and \( k'(\omega) \), the static parallel and perpendicular parts of reflectivity \( |R(0)| \) and \( |R'(0)| \), maximum peak values of \( R(\omega) \) and \( R'(\omega) \), anisotropy range for reflectivity, and the maximum peak values of the parallel and perpendicular components of the optical conductivity [i.e. \( \sigma(\omega)_{\text{max}} \) and \( \sigma'(\omega)_{\text{max}} \)].

<table>
<thead>
<tr>
<th>Compound</th>
<th>( n(0) )</th>
<th>( n'(0) )</th>
<th>( \Delta n(0) )</th>
<th>( n(\omega)_{\text{max}} )</th>
<th>( n'(\omega)_{\text{max}} )</th>
<th>( k(\omega)_{\text{max}} )</th>
<th>( k'(\omega)_{\text{max}} )</th>
<th>( R(0) )</th>
<th>( R'(0) )</th>
<th>( R(\omega)_{\text{max}} )</th>
<th>( R'(\omega)_{\text{max}} )</th>
<th>( \sigma(\omega)_{\text{max}} )</th>
<th>( \sigma'(\omega)_{\text{max}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>LiAlS(_2)</td>
<td>2.134</td>
<td>4.779</td>
<td>2.565</td>
<td>2.315</td>
<td>2.702</td>
<td>2.875</td>
<td>2.234</td>
<td>2.328</td>
<td>2.481</td>
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<tr>
<td>LiAlSe(_2)</td>
<td>2.179</td>
<td>4.100</td>
<td>2.490</td>
<td>2.265</td>
<td>2.615</td>
<td>2.798</td>
<td>2.184</td>
<td>2.348</td>
<td>2.514</td>
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<td>LiAlTe(_2)</td>
<td>3.06</td>
<td>4.86</td>
<td>3.45</td>
<td>3.13</td>
<td>3.54</td>
<td>3.78</td>
<td>2.85</td>
<td>2.89</td>
<td>3.21</td>
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<td>3.45</td>
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<td>3.78</td>
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<td>2.89</td>
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<td>LiGaTe(_2)</td>
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<td>10.19</td>
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<td>8.91</td>
<td>11.27</td>
<td>10.08</td>
<td>8.36</td>
<td>10.21</td>
<td>9.18</td>
<td>8.01</td>
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<td>LiInSe(_2)</td>
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<td>0.131</td>
<td>0.427</td>
<td>0.192</td>
<td>0.211</td>
<td>0.234</td>
<td>0.145</td>
<td>0.159</td>
<td>0.181</td>
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<td>0.234</td>
<td>0.145</td>
<td>0.159</td>
<td>0.181</td>
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</tbody>
</table>

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shift to lower energies when the anions are changed from the S to Te atoms as well as when the cations are changed from In to Al for these compounds. This shift of the $R(\omega)$ peak in the compounds to lower energies is reflected by the decrease in the energy bandgap when the cation is changed from S to Te and the anion is changed from Al to In. The calculated values of $R(\omega)$ at the zero frequency, the maximum values corresponding to the $R(\omega)$ and $R(\omega)$ spectra, and the anisotropy range of the optical reflectivity spectra are shown in Table 3. The anisotropy peak value (as shown in Fig. 7) of the optical reflectivity is negative, and high values of the reflectivity, $R(\omega)$, are observed to occur in the ultraviolet and visible portion of the electromagnetic spectra. Therefore, the LiMX$_2$ compounds could become interesting candidates for the Bragg’s reflectors.

The frequency-dependent optical conductivity, $\sigma(\omega)$, is calculated for the LiMX$_2$ (M = Al, Ga, In and X = S, Se, Te) compounds in the chalcopyrite phase. Similarly, the peak values of the parallel and perpendicular components $[\sigma_{||}(\omega), \sigma_{\perp}(\omega)]$, which are dependent on the frequency of the optical conductivity, are calculated and listed in Table 3. The threshold energies of the optical conductivity spectra corresponding to the LiAlS$_2$, LiAlSe$_2$, LiAlTe$_2$, LiGaS$_2$, LiGaSe$_2$, LiGaTe$_2$, LiInS$_2$, LiInSe$_2$, LiInTe$_2$, LiGaS$_2$, LiGaSe$_2$, LiGaTe$_2$, LiInS$_2$, LiInSe$_2$, LiInTe$_2$ compounds are shown in Table 3.
LiGaS$_2$, LiGaSe$_2$, LiGaTe$_2$, LiInS$_2$, LiInSe$_2$, and LiInTe$_2$ compounds are 4.08, 0.1, 2.1, 2.8, 1.4, 1.18, 2.08, 1.7, and 1.9, respectively. From Figure 8, it is observed that the optical conductivities initially increase gradually until the energies where the optical conductivities attain the maximum values. This is followed by the decrease of the magnitude of $\sigma(\omega)$ to low values at high energies where the peak values for both the $\sigma_\parallel(\omega)$ and $\sigma_\perp(\omega)$ components are calculated and displayed in Table 3.

4 Conclusions

Structural parameters are in good agreement with the available experimental and theoretical data. The LiAlTe$_2$ and LiGaTe$_2$ compounds show indirect bandgap situated at the $\Gamma$-symmetry point of the BZ using the EV-GGA potential. Bandgaps of the LiAlS$_2$, LiAlSe$_2$, LiGaS$_2$, LiGaSe$_2$, LiInS$_2$, LiInSe$_2$, and LiInTe$_2$ compounds show direct bandgap nature where the bandgap values decrease from the Al to In atoms and also from the S to Te atoms except for the LiAlSe$_2$, LiInSe$_2$, and LiGaTe$_2$ compounds. Compounds have mixed ionic-covalent bonding nature. Static refractive indices of the compounds are larger than 2, which indicate that the LiMX$_2$ compounds are important for the optoelectronic device applications where different peaks in the spectra are noticeable in the visible and ultraviolet portion of the electromagnetic spectra. The birefringence of the LiMX$_2$ compounds is high in the ultraviolet region, and the extinction coefficient of the compounds shows high absorption in the visible and ultraviolet region. In addition, the high peaks in the calculated absorption and optical reflectivity spectra lay in the visible and ultraviolet portion of the electromagnetic spectra, which suggests that the materials are ideal for various applications such as Bragg’s reflector and optical and optoelectronic devices.

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References