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Optical, electronic, and elastic properties of some $A^5B^6C^7$ ferroelectrics ($A=$Sb, Bi; $B=$Te, Se; $C=$I, Br, Cl): First principle calculation

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ABSTRACT
In present paper, we focus on the structural, mechanical, electronic, and optical properties for the $A^5B^6C^7$($A=$Sb, Bi; $B=$Te, Se; $C=$I, Br, Cl) compounds using the density functional methods in generalized gradient approximation. The lattice parameters, mechanical properties, electronic bands structures and the partial densities of states corresponding to the band structures, and optical properties are presented and analysed. Our structural estimation and some other results are in agreement with the available experimental and theoretical data.

KEYWORDS
Electronic properties; band structure; ferroelectrics

1. Introduction
The many $A^5B^6C^7$ ($A=$Sb, Bi; $B=$Te, Se; $C=$I, Br, Cl) compounds that are layered non-centrosymmetric materials have significant thermoelectric, photoelectric, and ferroelectric properties [1–5]. The large Rashba-type spin-orbit-coupling (SOC) in the bulk and surface electronic structure of these compounds has recently attracted great interest [6–10]. The Rashba effect can be utilized in important spintronics applications, such as the spin-based transistor [11]. The effects of large Rahba spin splitting in $A^5B^6C^7$ by angle-resolved photoemission spectroscopy (ARPES) has been observed [6,12–15].

The experimental studies and first principle calculations have increasingly been employed to explore the electronic and crystal structure of these compounds. Zhuang et al. [10] investigated the Rashba spin splitting in the spin orbit coupling (SOC) band structure, density of state and phonon properties of single layer SbTel using VASP code. Akrapet et al. [15] investigated the optical properties and Raman spectra of BiTeBr and BiTeCl single crystal using chemical vapor transport and topotactic methods. Fiedler et al. [9] investigated the surface structural and electronic properties of the semiconductors BiTeX ($X=$Cl, Br, I) using the various techniques. Moreschiniet et al. [16] investigated the surface states using the QUANTUM-ESPRESSO package. Dubeyet et al. [17] observed that SbTel showed metallic behavior from 4 K to 300 K and semiconducting behavior at higher temperature.
Landolt et al. [18] investigated the three dimensional bulk states and the two dimensional surface states using the GGA. Kulbachinski et al. [19] investigated the thermoelectric and galvanomagnetic properties using the Bridgman method. Ma et al. [20] examined the energetic stability electronic and phonon properties of BiTeX (X = Br, I) monolayers using ab initio calculations. Zhu et al. [21] calculated the electronic band structure of BiTeCl in the absence of spin orbit coupling using the WIEN2k package.

In the present work, we aimed at providing some additional information to the existing data on the physical properties of A5B6C7 compounds by using ab initio total energy calculations, and we especially focused on the electronic, mechanical, and optical properties. To our knowledge, the mechanical properties for SbTeI and BiSI compounds, optical properties of dielectric functions (except for the part real and imaginary of BiSI) have not been reported in detail for these compounds so far.

2. Method of calculation

In all of our calculations that were performed using the ab-initio total-energy and molecular-dynamics program VASP (Vienna ab-initio simulation program) [22–25] that was developed within the density functional theory (DFT) [26], the exchange-correlation energy function is treated within the GGA (generalized gradient approximation) by the density functional of Perdew et al. [27]. The potentials used for the GGA calculations take into account the 6s^26p^3 valence electrons of each Bi-, 5s^25p^3 valence electrons of each Sb-, 5s^25p^4 valence electrons of each Te-, 3s^23p^4 valence electrons of each S-, 3s^23p^5 valence electrons of each Cl-, and 4s^24p^5 valence electrons of each Br-atoms. When including a plane-wave basis up to a kinetic-energy cutoff equal to 10.72 Ha (for SbTeI), 12.85 Ha (for BiTeI), 12.87 Ha (for BiTeCl), 22.18 Ha (for BiTeBr), and 20.47 Ha (for BiSI), the properties investigated in this work are well converged. The Brillouin-zone integration was performed using special k points sampled within the Monkhorst-Pack scheme [28]. We found that a mesh of 11 × 11 × 4, 8 × 8 × 4, 9 × 9 × 3, 11 × 11 × 6, and 8 × 16 × 7 k points for SbTeI, BiTeI, BiTeCl, BiTeBr and BiSI, respectively, was required to describe the structural, mechanical, electronic, and optical properties. This k-point mesh guarantees a violation of charge neutrality less than 0.008e. Such a low value is a good indicator for an adequate convergence of the calculations.

The positions corresponding to the A5B6C7 (A = Sb, Bi; B = Te, Se; S; C = I, Br, Cl) compounds have been obtained from experimental data [30–39]. The atomic positions belonging to these compounds are given in Table 1. The crystal structures of BiTeI and BiTeBr compounds are the same. Both of these compounds crystallize in a trigonal structure with space groups P3m1 (156), and the unit cell of the crystal structures contains 1 molecule and 3 atoms. BiTeCl has a hexagonal crystal structure with space groups P6_3mc (186), and the unit cell of the crystal structure contains 2 molecules and 6 atoms. SbTeI and BiSI compounds crystallize in monoclinic and orthorhombic structures with space groups C2/m (12) and Pnma(62), respectively. The unit cell each of these compounds contains 4 molecules and 12 atoms.

3. Results and discussion

We have used the experimental structural parameter in the first step of our calculation, but these values may not always give the correct result. Therefore, the geometric optimization
process is performed to detect that the structure is the correct structure. The lattice parameters obtained as a result of optimization are given in Table 1 along with the experimental and theoretical values, and these parameters are used for the electronic, mechanical, and optical calculations. The obtained lattice parameters for the A₅B₆C₇ (A = Sb, Bi; B = Te, Se; S; C = I, Br, Cl) compounds are in agreement with the experimental and theoretical values [29, 30, 33–38].

The elastic constants calculated with the strain-stress relationship [41] for A₅B₆C₇ compounds are given in Table 2 along with the theoretical values. As can be seen in Table 2, the value of the calculated elastic constants for BiTeI compound is in good agreement with the theoretical values. However, the value of the calculated elastic constant C₃₃ for BiTeBr is higher than the theoretical value, but the calculated C₃₃ (C₄₄) value for BiTeCl is lower (higher) than the theoretical value. It is seen that all the

<table>
<thead>
<tr>
<th>Lattice Material</th>
<th>a (Å)</th>
<th>b (Å)</th>
<th>c (Å)</th>
<th>V₀ (Å³)</th>
<th>E₀ (eV)</th>
<th>Refs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trigonal P3m1 (156) BiTeI</td>
<td>4.425</td>
<td>7.227</td>
<td>122.53</td>
<td>1.24</td>
<td>Present</td>
<td></td>
</tr>
<tr>
<td>BiTeBr</td>
<td>4.339</td>
<td>6.854</td>
<td>111.81</td>
<td></td>
<td>Exp. [29]</td>
<td></td>
</tr>
<tr>
<td>BiTeCl</td>
<td>4.437</td>
<td>7.433</td>
<td>127.04</td>
<td>0.43</td>
<td>PAW-PBE [30]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4.284</td>
<td>7.021</td>
<td>111.63</td>
<td>0.21</td>
<td>PAW-PBE-D2 [30]</td>
<td></td>
</tr>
<tr>
<td>Hexagonal P6₃mc (186) BiTeI</td>
<td>4.328</td>
<td>6.906</td>
<td>115.79</td>
<td>1.09</td>
<td>Present</td>
<td></td>
</tr>
<tr>
<td>BiTeBr</td>
<td>4.351</td>
<td>7.064</td>
<td>115.79</td>
<td>1.09</td>
<td>Exp. [31]</td>
<td></td>
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<tr>
<td>BiTeCl</td>
<td>4.266</td>
<td>6.486</td>
<td>102.25</td>
<td>0.8</td>
<td>Exp. [32]</td>
<td></td>
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<tr>
<td>Monoclinic C2/m (12) SbTeI</td>
<td>4.213</td>
<td>12.531</td>
<td>1.2</td>
<td>UPPW-PBE [33]</td>
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<td></td>
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<tr>
<td></td>
<td>4.903</td>
<td>4.299</td>
<td>9.778</td>
<td>472.09</td>
<td>0.89 eV (l)</td>
<td>Present</td>
</tr>
<tr>
<td>Orthorhombic Pnma (62) BiSI</td>
<td>8.926</td>
<td>4.207</td>
<td>11.023</td>
<td>413.92</td>
<td>1.88 (l)</td>
<td>Exp. [36]</td>
</tr>
<tr>
<td></td>
<td>8.45</td>
<td>1.139</td>
<td>10.147</td>
<td>354.88</td>
<td>1.78 (l) 1.82 (D)</td>
<td>UPPW-PBE [38]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>8.44</td>
<td>4.13</td>
<td>10.26</td>
<td>1.57 (l)</td>
<td>1.59</td>
</tr>
</tbody>
</table>

Table 1. The calculated equilibrium lattice parameters (a, b, and c in Å) and electronic band gaps together with the theoretical and experimental values for A₅B₆C₇ (A = Sb, Bi; B = Te, Se; S; C = I, Br, Cl) compounds.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Refs.</th>
<th>C₁₁</th>
<th>C₁₂</th>
<th>C₁₃</th>
<th>C₁₅</th>
<th>C₂₂</th>
<th>C₂₃</th>
<th>C₂₅</th>
<th>C₃₃</th>
<th>C₃₅</th>
<th>C₄₄</th>
<th>C₄₆</th>
<th>C₅₅</th>
<th>C₆₆</th>
</tr>
</thead>
<tbody>
<tr>
<td>BiTeI</td>
<td>Present</td>
<td>57.8</td>
<td>16.1</td>
<td>25.5</td>
<td>46.2</td>
<td>20.9</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BiTeBr</td>
<td>Present</td>
<td>60.4</td>
<td>14.1</td>
<td>20.2</td>
<td>42</td>
<td>24.3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BiTeCl</td>
<td>Present</td>
<td>59.8</td>
<td>18.4</td>
<td>23.2</td>
<td>54.8</td>
<td>20.6</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SbTeI</td>
<td>Present</td>
<td>59.3</td>
<td>14.9</td>
<td>13.1</td>
<td>28.6</td>
<td>14.9</td>
<td></td>
<td></td>
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<tr>
<td>BiSI</td>
<td>Present</td>
<td>74.2</td>
<td>21.4</td>
<td>32.4</td>
<td>55.8</td>
<td>26.5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

Table 2. The calculated elastic constants (in GPa) for A₅B₆C₇ (A = Sb, Bi; B = Te, Se; S; C = I, Br, Cl) compounds.
compounds under zero pressure provide the mechanical stability criteria [42–46]. The elastic constants $C_{11}$, $C_{22}$, and $C_{33}$ measure the a-, b-, and c-direction resistance to linear compression, respectively. The $C_{11}$ value for BiTeI, BiTeBr, and BiTeCl compounds is higher than the $C_{33}$ value. Therefore, the a-direction of these compounds is less compressible. The $C_{22}$ value for the BiSI compound is higher than the $C_{11}$ and $C_{33}$ values while the $C_{33}$ value for SbTeI compound is higher than $C_{11}$ and $C_{33}$ values. At that, the c-direction for SbTeI and the b-direction for BiSI are less compressible. $C_{44}$, $C_{55}$, and $C_{66}$ values show the shear distortion resistance in the (100), (010), and (001) plane, respectively. The SbTeI compound from these compounds has higher $C_{44}$ and $C_{66}$ values. BiSI compound also has a higher $C_{33}$ value.

The other polycrystalline elastic properties (Young’s modulus, Poisson’s ratio, sound velocities, and Debye temperature) from the polycrystalline bulk modulus and isotropic shear modulus obtained by using the Voigt- Reuss-Hill (VRH) approach [47–49] have been calculated, and have been given in Table 3 along with the theoretical values. It is seen that the values of BiTeI and BiTeBr are in good agreement with the theoretical values, but the values of BiTeCl are not in good agreement with the theoretical values (except for the bulk modulus). The isotropic shear modulus and bulk modulus are a measure of the hardness of a solid. The bulk modulus and isotropic shear modulus for BiSI compound are higher than the other composite values. Young’s modulus is defined as the ratio of stress and strain, and used to provide a measure of the stiffness of the solid. Here, the most high Young’s modulus belongs to BiSI compound. Therefore, this compound is harder than the other compounds. The value of the Poisson’s ratio is indicative of the degree of directionality of the covalent bonds. The value of Poisson’s ratio is small ($\nu = 0.1$) for covalent materials, whereas for ionic materials a typical value of $\nu$ is 0.25 [50–51]. As can be seen in Table 3, the ionic contribution to inter atomic bonding for these compounds is dominant. According to the criterion in refs. [52, 53], a material is brittle (ductile) if the $B / G$ ratio is less (high) than 1.75. The value of the $B / G$ of BiTeI, BiTeCl, and BiSI compounds is higher than 1.75. Hence, these compounds behave in a ductile manner. The value of the $B / G$ of BiTeBr and SbTeI compounds is also less than 1.75. Hence, these compounds behave in a brittle manner. The elastic anisotropy is given by the percentage of anisotropy in the compression ($A_B$) and shear ($A_G$). For crystals, these values can range from zero (isotropic) to 100% representing the maximum anisotropy [50, 54,55]. The SbTeI among these compounds has high shear and bulk anisotropies.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Reference</th>
<th>B (GPa)</th>
<th>G (GPa)</th>
<th>E (GPa)</th>
<th>$\nu$</th>
<th>$B/G$</th>
<th>$A_B$</th>
<th>$A_G$</th>
<th>$A^U$</th>
<th>$\nu_t$</th>
<th>$\nu_l$</th>
<th>$\nu_m$</th>
<th>$\theta_D$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BiTeI</td>
<td>Present</td>
<td>32.8</td>
<td>18.1</td>
<td>45.9</td>
<td>0.27</td>
<td>1.81</td>
<td>0.02</td>
<td>3.58</td>
<td>0.37</td>
<td>1697</td>
<td>3010</td>
<td>1888</td>
<td>163</td>
</tr>
<tr>
<td></td>
<td>UPPW-PBE  [33]</td>
<td>30.0</td>
<td>18.8</td>
<td>46.6</td>
<td>0.24</td>
<td>1.6</td>
<td>0.72</td>
<td>14.75</td>
<td>1.74</td>
<td>1653</td>
<td>2831</td>
<td>1834</td>
<td>163</td>
</tr>
<tr>
<td>BiTeBr</td>
<td>Present</td>
<td>33.8</td>
<td>19.6</td>
<td>49.3</td>
<td>0.26</td>
<td>1.72</td>
<td>0.002</td>
<td>0.51</td>
<td>1.35</td>
<td>13.05</td>
<td>1537</td>
<td>2607</td>
<td>1703</td>
</tr>
<tr>
<td></td>
<td>UPPW-PBE  [33]</td>
<td>24.0</td>
<td>13.5</td>
<td>38.3</td>
<td>0.23</td>
<td>1.54</td>
<td>6.1</td>
<td>13.05</td>
<td>1.63</td>
<td>1537</td>
<td>2607</td>
<td>1703</td>
<td>155</td>
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<tr>
<td>BiTeCl</td>
<td>Present</td>
<td>41.2</td>
<td>22.8</td>
<td>57.9</td>
<td>0.27</td>
<td>1.83</td>
<td>0.19</td>
<td>4.23</td>
<td>0.45</td>
<td>1983</td>
<td>3529</td>
<td>2207</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>UPPW-PBE  [33]</td>
<td>42.9</td>
<td>7.0</td>
<td>20.0</td>
<td>0.42</td>
<td>6.1</td>
<td>14.37</td>
<td>49.4</td>
<td>10.1</td>
<td>1047</td>
<td>2856</td>
<td>1189</td>
<td>111</td>
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<tr>
<td>SbTeI</td>
<td>Present</td>
<td>30.2</td>
<td>22.4</td>
<td>53.9</td>
<td>0.2</td>
<td>1.35</td>
<td>14.24</td>
<td>13.2</td>
<td>1.85</td>
<td>2057</td>
<td>3368</td>
<td>2272</td>
<td>199</td>
</tr>
<tr>
<td>BiSI</td>
<td>Present</td>
<td>42.0</td>
<td>24.0</td>
<td>60.5</td>
<td>0.26</td>
<td>1.75</td>
<td>0.83</td>
<td>9.17</td>
<td>1.03</td>
<td>2016</td>
<td>3540</td>
<td>2241</td>
<td>205</td>
</tr>
</tbody>
</table>
A concept of the universal anisotropy index, which is another way of measuring the elastic anisotropy, was introduced by Ranganathan et al. \[56,33\]:

\[
A^U = 5 \frac{G_V}{G_R} + \frac{B_V}{B_R} - 6
\]  

Here, \(A^U = 0\) represents locally isotropic crystals and \(A^U > 0\) denotes the extent of crystal anisotropy. SbTeI compound has strong anisotropy because the SbTeI among these compounds has a high \(A^U\) value. The Debye temperature and sound velocity \[57–59\] calculated for these compounds are given in Table 2 along with the theoretical values. The least Debye temperature belongs to the SbTeI compound, but the values of other compounds are also close to this value. Usually, the Debye temperature is low for soft materials, but is high for rigid materials. Consequently, these compounds can be called soft materials. The highest Debye temperature among these compounds belongs to the BiSI compound, and this compound is rigid material accord to the other compounds.

The calculated band structures and partial densities of states of \(A^5B^6C^7\) compounds along high symmetry directions using the lattice constants obtained are shown in Fig. 1. The Fermi energy level has been taken as zero. As can be seen in Fig. 1, BiTel, BiTeCl, SbTeI, and BiSI compounds have indirect band gap, which are 1.24 eV (from the nearly A point between A and T to A high symmetry point), 1.38 eV (from the nearly G point between G and K to G point), 0.89 eV (from the nearly G point between G and Z to Z point), and 1.88 eV (from nearly the Y point between S and Y point to nearly the T point between T and Z point), respectively. BiTeBr compound also has a direct band gap, which is 1.09 eV (ahigh symmetry point). The obtained band gap values for these compounds have been summarized in Table 1 along with the experimental and theoretical values. The obtained band gap value for BiTeI compound is too high for the experimental and theoretical values \[6, 29–31\], but this value is a little higher than the theoretical value \[33\]. The values of BiTeBr, BiTeCl, and BiSI compounds are in agreement with the experimental and theoretical values \[33, 36, 38–40\]. Unfortunately, there are no theoretical and experimental results for comparing with the band gap value of SbTeI compound. The materials with the narrow band gap are important for mid-infrared optoelectronic applications \[60–61\]. In this respect, the semiconductors with the narrow band gap from these compounds can be alternative for mid-infrared applications. The density of states of these compounds is similar to one another as shown in Fig. 1. In this figures, the lowest valance bands for these compounds are dominated by d states that occur between approximately \(-24\) and \(-22\) eV. The mid-level valance bands are also dominated by s states that occur between approximately \(-15\) and \(-8\) eV. The highest occupied valance bands and the lowest unoccupied conduction bands are dominated by p states. The d and s states also contributeto the highest occupied valance and the lowest unoccupied conduction bands, but the values of the density of states of these states are rather small compared to p states. Therefore, the ionic bonding structure for these compounds dominates because of the p states that play a role in the transmission.

We first calculated the real and imaginary parts of \(\varepsilon(\omega) = \varepsilon_1(\omega) - i\varepsilon_2(\omega)\) for the \(A^5B^6C^7\) compounds (except for the part real and imaginary of BiSI) along the x- and z- direction using Kramers-Kroning transformation \[62\]. Figure 2 shows the real and imaginary of \(\varepsilon(\omega)\) together with the energy loss function. The results obtained showa manner similar to our recent works \[63,64\]. The \(\varepsilon_1\) behaves mainly as a classical oscillator. The \(\varepsilon_1\) parts (for \(d\varepsilon_1\)
Figure 1. Energy band structures and projected density of states for (a) BiTeI, (b) BiTeBr, (c) BiTeCl, (d) SbTeI, and (e) BiSI compounds.
Figure 2. Energy spectra of the dielectric function $\varepsilon = \varepsilon_1 - i\varepsilon_2$ and energy-loss function (L) along the x- and z-axes for (a) BiTeI, (b) BiTeBr, (c) BiTeCl, (d) SbTeI, and (e) BiSI compounds.
The peaks of the $e_2$ parts are related to the optical transitions from the valance bands to the conduction band. The maximum peak values of $e_{2x}^2 (e_{2z}^2)$ for BiTeI, BiTeBr, BiTeCl, SbTeI, and BiSI compounds around 2.85 (3.70) eV, 2.55...
Table 4. Some of principal features and singularities of the linear optical responses for A\(^5\)B\(^6\)C\(^7\) (A = Sb, Bi; B = Te, Se; C = I, Br, Cl) compounds.

<table>
<thead>
<tr>
<th>Material</th>
<th>(\varepsilon_1) (eV)</th>
<th>(\varepsilon_1) / (d\varepsilon_1 / dE &lt; 0)</th>
<th>(\varepsilon_1) / (d\varepsilon_1 / dE &gt; 0)</th>
<th>(\varepsilon_2) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BiTeI</td>
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<td>7.45</td>
<td>6.37</td>
<td>16.44</td>
</tr>
<tr>
<td>BiTeBr</td>
<td>3.70</td>
<td>8.14</td>
<td>6.26</td>
<td>16.39</td>
</tr>
<tr>
<td>BiTeCl</td>
<td>2.96</td>
<td>6.05</td>
<td>8.48</td>
<td>5.28</td>
</tr>
<tr>
<td>SbTeI</td>
<td>3.20</td>
<td>9.31</td>
<td>6.88</td>
<td>15.83</td>
</tr>
<tr>
<td>SbTeBr</td>
<td>3.62</td>
<td>7.86</td>
<td>6.03</td>
<td>17.26</td>
</tr>
<tr>
<td>BiSI</td>
<td>4.93</td>
<td>8.75</td>
<td>6.32</td>
<td>17.61</td>
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</tbody>
</table>

As can be seen in Table 4, the \(\varepsilon_1\) \(\varepsilon_2\) values of BiSI compound are in agreement with the theoretical values [39]. The function \(L(\omega)\) describes the energy loss of fast electrons traversing the material. The sharp maxima in the energy-loss function are associated with the existence of plasma oscillations [65]. As can be seen in Figure 2, the \(L_\alpha(\omega)\) curves have a maximum near 17.47 \(16.61\) eV for BiTel, 18.01 \(17.96\) eV for BiTeBr, 18.37 \(17.62\) eV for BiTeCl, 17.44 \(17.41\) eV for SbTeI, and 18.02 \(17.67\) eV for BiSI. The known sum rules can be used to determine some quantitative parameters, as well as the effective number of the valence electrons per unit cell \(N_{\text{eff}}\) and the effective optical dielectric constant \(\varepsilon_{\text{eff}}\) [66]. The calculated effective number of valence electrons \(N_{\text{eff}}\) and the effective dielectric constant \(\varepsilon_{\text{eff}}\) are given in Fig. 3. The effective number of valance electrons per unit cell, \(N_{\text{eff}}\) (contributing in the interband transitions), reaches the saturation value at energies above 25 eV. This means that deep-lying valence orbitals participate in the interband transitions as well. The effective optical dielectric constant \(\varepsilon_{\text{eff}}\) reaches a saturation value at approx. 10 eV. This means that the greatest contribution to \(\varepsilon_{\text{eff}}\) arises from interband transitions between 0.5 eV and 10 eV (see Fig. 3).

Conclusion

The ternary chalcohalides formed from the group 5-6-7 elements (A\(^5\)B\(^6\)C\(^7\) where A = Bi, Sb; B = S, Se, Te; C = I, Br, Cl) constitute a class of materials exhibiting a wide range of interesting and potentially useful semiconducting and ferroelectric properties. Some compounds of this class are topological insulators (BiTel, SbTeI, and BiSeI) and have recently been attracting a great deal of interest as a potential spintronic material due to the emergence of giant Rashba-type spin splitting in their band structures. In the present paper, we focus on general principles governing the emergence of valence electronic states in different A\(^5\)B\(^6\)C\(^7\) and their electronic band structure, optical, and elastic properties for the ABC compounds using the density functional methods in a generalized gradient approximation. The lattice parameters of considered compounds have been calculated. The second-order elastic constants have been calculated, and the other related quantities such as Young’s modulus, shear modulus, Poisson’s ratio, anisotropy factor, sound velocities, and Debye temperature have also been estimated in the present work. The electronic band structures and the partial densities of

(2.96) eV, 3.34 (4.26) eV, 3.33 (2.71) eV, and 3.30 (3.30) eV, respectively. As can be seen in Table 4, the \(\varepsilon_1\) \(\varepsilon_2\) values of BiSI compound are in agreement with the theoretical values [39]. The function \(L(\omega)\) describes the energy loss of fast electrons traversing the material. The sharp maxima in the energy-loss function are associated with the existence of plasma oscillations [65]. As can be seen in Figure 2, the \(L_\alpha(\omega)\) curves have a maximum near 17.47 (16.61) eV for BiTel, 18.01 (17.96) eV for BiTeBr, 18.37 (17.62) eV for BiTeCl, 17.44 (17.41) eV for SbTeI, and 18.02 (17.67) eV for BiSI. The known sum rules can be used to determine some quantitative parameters, as well as the effective number of the valence electrons per unit cell \(N_{\text{eff}}\) and the effective optical dielectric constant \(\varepsilon_{\text{eff}}\) [66]. The calculated effective number of valence electrons \(N_{\text{eff}}\) and the effective dielectric constant \(\varepsilon_{\text{eff}}\) are given in Fig. 3. The effective number of valance electrons per unit cell, \(N_{\text{eff}}\) (contributing in the interband transitions), reaches the saturation value at energies above 25 eV. This means that deep-lying valence orbitals participate in the interband transitions as well. The effective optical dielectric constant \(\varepsilon_{\text{eff}}\) reaches a saturation value at approx. 10 eV. This means that the greatest contribution to \(\varepsilon_{\text{eff}}\) arises from interband transitions between 0.5 eV and 10 eV (see Fig. 3).
states corresponding to the band structures are presented and analyzed. The real and imaginary parts of dielectric functions and hence the optical constant such as energy-loss function, the effective number of valance electrons and the effective optical dielectric constant are calculated. Our structural estimation and some other results are in agreement with the available experimental and theoretical data.

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