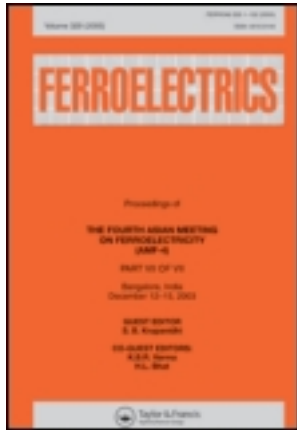


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# Optical Properties and Electronic Band Structure of Topological Insulators (on $A_2^V B_3^VI$ Compound Based)

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*We have performed a first principles study of structural, electronic, and optical properties of rhombohedral  $Sb_2Te_3$  and  $Bi_2Te_3$  compounds using the density functional theory within the local density approximation. The lattice parameters, bulk modulus, and its pressure derivatives of these compounds have been obtained. The linear photon-energy dependent dielectric functions and some optical properties such as the energy-loss function, the effective number of valance electrons and the effective optical dielectric constant are calculated and presented in the study.*

**Keywords:** Ab initio calculation; electronic structure; optical properties

## 1. Introduction

$Sb_2Te_3$  and  $Bi_2Te_3$ , the members of compounds with the general formula  $A_2^V B_3^VI$  ( $A = Bi, Sb$  and  $B = S, Se, Te$ ), are narrow-band gap semiconductors with rhombohedral layered crystal structure.  $Sb_2Te_3$  and  $Bi_2Te_3$  are well-known topological insulators [1–7], extraordinary thermoelectric materials at ambient temperature [8] and the possible topological superconductors [9] with surface states consisting of a single Dirac cone at the  $\Gamma$ . All of these have made  $A_2^V B_3^VI$  compounds as the subject of intensive investigation both in fundamental and applied research. These compounds possess the rhombohedral crystal structure with five atoms per unit cell belonging to the space group  $D_{3d}^5(R\bar{3}m)$ .  $Sb_2Te_3$  and  $Bi_2Te_3$  can be used for many different applications such as power generation and cooling devices [10]. Thermoelectric power generators and cooler have many advantages over conventional refrigerators and power generators such as long life, no moving parts, no green house gases, no noise, low maintenance and high reliability [11–13].

In the past, some detailed works [6, 7, 14, 15] have been carried out on the structural and electronic properties of these compounds. Zhang et al. [6] study in detail the topological nature and the surface states of this family of compounds using the fully self-consistent ab initio calculations in the framework of density functional theory. Zhang et al. [7] focused on layered, stoichiometric crystals  $Sb_2Te_3$ ,  $Sb_2Se_3$ ,  $Bi_2Te_3$  and  $Bi_2Se_3$  using ab initio calculations in the framework of the Perdew-Burke-Ernzerhof type generalized gradient

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approximation of the density functional theory. Wang et al. [14] calculated the electronic structures of  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  crystals using the first-principles full potential linearized augmented plane-wave method. Yavorsky et al. [15] performed calculations of the electronic structures of  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  compounds by means of the screened Korringa-Kohn-Rostoker (KKR) Green's function method in the atomic sphere approximation (ASA) within local density approximation of the density functional theory. Choi et al. [16] reported the crystal growth and ferromagnetic (FM) properties of Mn-doped  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  bulk crystals.

As far as we know, no ab initio general potential calculations of the density of state, charge density and the optical properties of the  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  have been reported in detail. In the present work, we have investigated the structural, electronic, and photon energy-dependent optical properties of the  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  crystals. The method of calculation is given in Section 2; the results are discussed in Section 3. Finally, the summary and conclusion are given in Section 4.

## 2. Method of Calculation

Our calculations have been performed using the density functional formalism and local density approximation (LDA) [17] through the Ceperley and Alder functional [18] as parameterized by Perdew and Zunger [19] for the exchange-correlation energy in the SIESTA code [20, 21]. This code calculates the total energies and atomic forces using a linear combination of atomic orbitals as the basis set. The basis set is based on the finite range pseudoatomic orbitals (PAOs) of the Sankey-Niklewsky type [22], generalized to include multiple-zeta decays.

The interactions between electrons and core ions are simulated with separable Troullier-Martins [23] norm-conserving pseudopotentials. We have generated atomic pseudopotentials separately for atoms, Sb, Bi and Te by using the  $5s^25p^3$ ,  $6s^26p^3$  and  $5s^25p^4$  configurations, respectively. The cut-off radii for present atomic pseudopotentials are taken as  $s$ : 3.82 au,  $p$ : 2.71 au, 2.92 au for the  $d$  and  $f$  channels of Bi,  $s$ :3.62 au,  $p$ :2.40 au, 2.78 au for the  $d$  and  $f$  channels of Te and 2.35 for the  $s$ ,  $p$ ,  $d$  and  $f$  channels of Sb.

Siesta calculates the self-consistent potential on a grid in real space. The fineness of this grid is determined in terms of an energy cut-off  $E_c$  in analogy to the energy cut-off when the basis set involves plane waves. Here by using a double-zeta plus polarization (DZP) orbitals basis and the cut-off energies between 100 and 500  $Ry$  with various basis sets, we found an optimal value of around 425  $Ry$  for  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$ . For the final computations, 54  $k$ -points for  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  were enough to obtain the converged total energies  $\Delta E$  to about 1meV/atoms.

## 3. Results and Discussion

### 3.1 Structural Properties

All physical properties are related to the total energy. For instance, the equilibrium lattice constant of a crystal is the lattice constant that minimizes the total energy. If the total energy is calculated, any physical property related to the total energy can be determined.

For  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$ , structures which are rhombohedral are considered. The equilibrium lattice parameters, the bulk modulus, and its pressure derivative have been computed minimizing the crystal's total energy calculated for the different values of lattice constant

**Table 1**

The calculated equilibrium lattice parameters ( $a$  and  $c$ ), bulk modulus ( $B$ ), and the pressure derivative of bulk modulus ( $B'$ ), together with the theoretical and previous experimental values for  $Sb_2Te_3$  and  $Bi_2Te_3$

Material	Reference	$a$ (Å)	$c$ (Å)	$B$ (GPa)	$B'$ (GPa)
$Sb_2Te_3$	Present (LDA-SIESTA)	4.256	30.397	64.03	4.94
	Theory (GGA-FLEUR) <sup>a</sup>	4.440	30.290		
	Experimental <sup>b</sup>	4.250	30.350		
$Bi_2Te_3$	Present (LDA-SIESTA)	4.383	30.487	46.05	4.56
	Theory (GGA-FLUER) <sup>a</sup>	4.530	30.630		
	Experimental <sup>b</sup>	4.383	30.487		

<sup>a</sup>Reference [14].

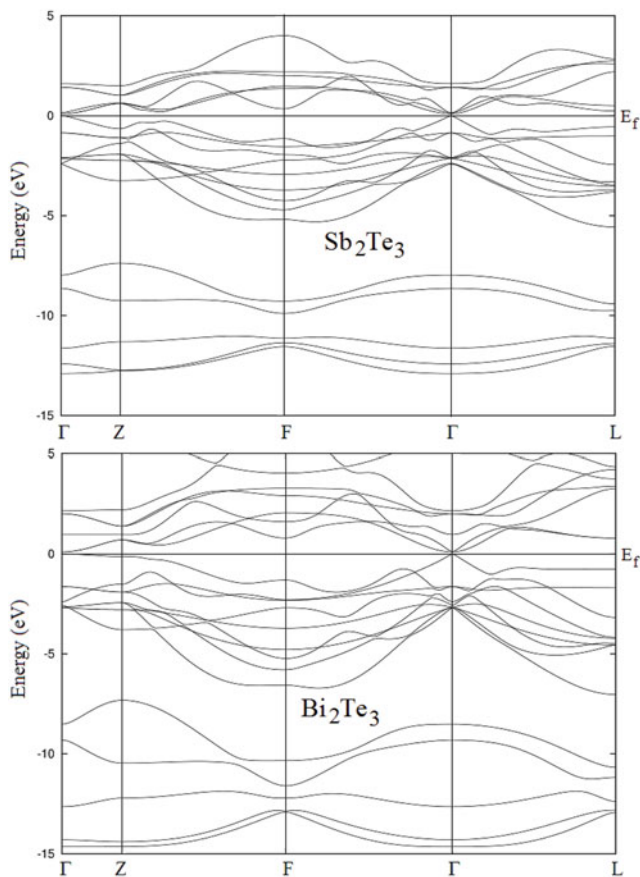
<sup>b</sup>Reference [25].

by means of Murnaghan's equation of states (eos) [24], and the results are shown in Table 1 along with the experimental and theoretical values. The lattice constants for  $Sb_2Te_3$  and  $Bi_2Te_3$  compounds are found to be  $a = 4.256$  Å,  $b = 30.397$  Å and  $a = 4.383$  Å,  $b = 30.487$  Å, respectively. The lattice parameters obtained are in a good agreement with the experimental and theoretical values [25, 14]. In all our calculations, we have used the computed lattice constants. In the present case, the calculated bulk moduli for  $Sb_2Te_3$  and  $Bi_2Te_3$  are 64.03 and 46.05 GPa, respectively. Unfortunately, there are no theoretical and experimental results for comparing with calculated bulk modulus.

### 3.2. Electronic Properties

**3.2.1. Density of States and Band Structure.** For a better understanding of the electronic and optical properties of  $Sb_2Te_3$  and  $Bi_2Te_3$ , the investigation of the electronic band structure would be useful. The electronic band structures of rhombohedral  $Sb_2Te_3$  and  $Bi_2Te_3$  single crystals have been calculated along high symmetry directions in the first Brillouin zone (BZ) using the results of SIESTA calculations. The band structures were calculated along the special lines connecting the high-symmetry points  $\Gamma(0,0,0)$ , Z ( $\Pi, \Pi, \Pi$ ), F ( $\Pi, \Pi, 0$ ), L ( $\Pi, 0, 0$ ) for  $Sb_2Te_3$  and  $Bi_2Te_3$  in the k-space. The results of the calculation are shown in Fig. 1 for these single crystals.

The energy band structures calculated using LDA for  $Sb_2Te_3$  and  $Bi_2Te_3$  are shown in Fig. 1. As can be seen in Fig. 1, the  $Sb_2Te_3$  and  $Bi_2Te_3$  compounds have a direct band gap semiconductor with the values 0.093 eV and 0.099 eV, respectively. The top of the valence band and the bottom of the conduction band for both compounds are positioned at the  $\Gamma$  point of BZ. In conclusion, our band gap values obtained are in good agreement with theoretical values and the band gaps have the same character with given in Ref. [6, 7]. Band structures of  $Sb_2Te_3$  and  $Bi_2Te_3$  single crystals are compared, and the band structures of these crystals are highly similar to one another. Thus, on formation of the band structures of  $Sb_2Te_3$  and  $Bi_2Te_3$  the 5s 5p orbitals of Te atoms are more dominant than 5s 5p and 6s 6p orbitals of Sb and Bi atoms.  $Bi_2Te_3$  and  $Sb_2Te_3$  also have the particular properties in which the surface states located around the  $\Gamma$  point; both conduction band minimum and valence band maximum of bulk states are located around  $\Gamma$  point, too. In other words, for the low energy range, the surface states and bulk states were not separated in the momentum space (see Fig. 2). From

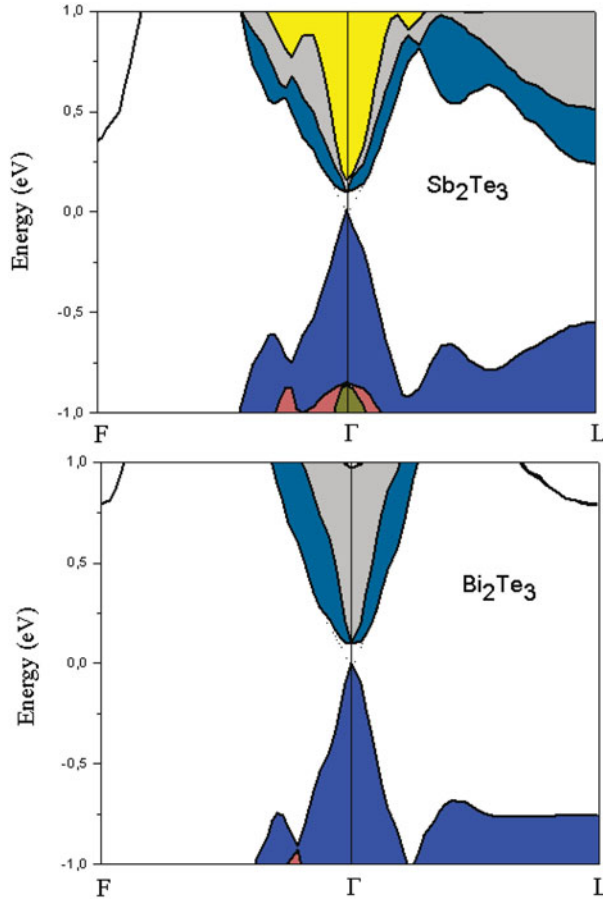


**Figure 1.** Energy band structure for  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  (Color figure available online).

our data one clearly see that Dirac cone that intersects at the Fermi level at  $0.09 \text{ \AA}$  which agrees well with other results [7, 9].

The total and partial densities of states of  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  are illustrated in Fig. 3. As you can see, from this figure, the lowest valence bands occur between about  $-14$  and  $-12 \text{ eV}$  are dominated by Sb 5s and Bi 6s states while valence bands occur between about  $-12$  and  $-10 \text{ eV}$  are dominated by Te 5s states. The highest occupied valence bands are essentially dominated by Te 5p states. The 5p (6p) states of Sb (Bi) atoms are also contributing to the valence bands, but the values of densities of these states are so small compared to Te 5p states. The lowest unoccupied conduction bands just above Fermi energy level are dominated by Sb 5p and Bi 6p states. The 5p states of Te atoms are also contributing to the conduction bands, but the values of densities of these states are so small compared to Sb 5p and Bi 6p states.

**3.2.2. Charge Density.** The three-dimensional valance charge density distribution of  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  compounds in the plane containing Sb-Te and Bi-Te bonds is illustrated in Fig. 4 and Fig. 5. Examination of the nature of chemical bonding, especially the distribution of valance charges between atoms, is necessary to explain the overall shape.

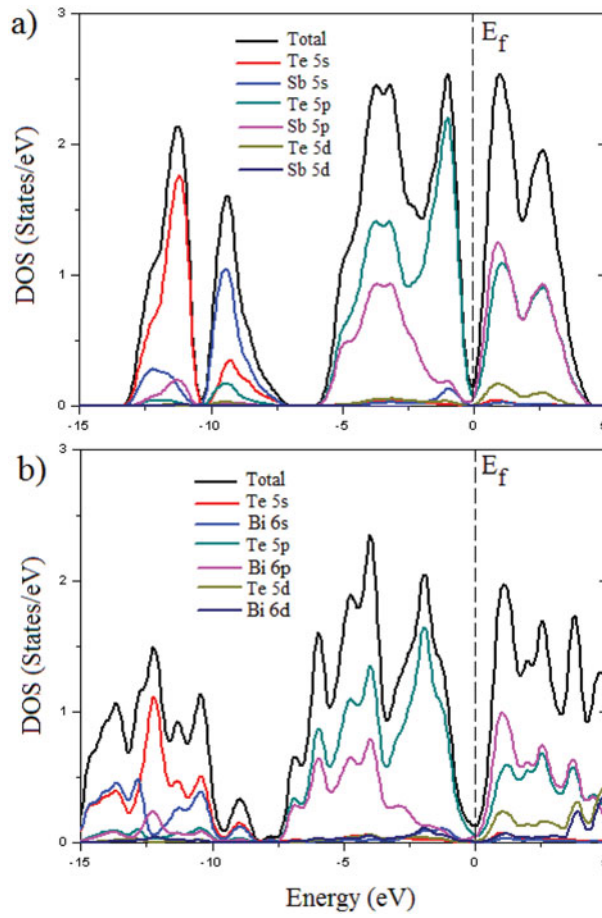


**Figure 2.** Schematic band structure of the  $Sb_2Te_3$  and  $Bi_2Te_3$  near  $\Gamma$  point of the first Brillouin zone (BZ) (Color figure available online).

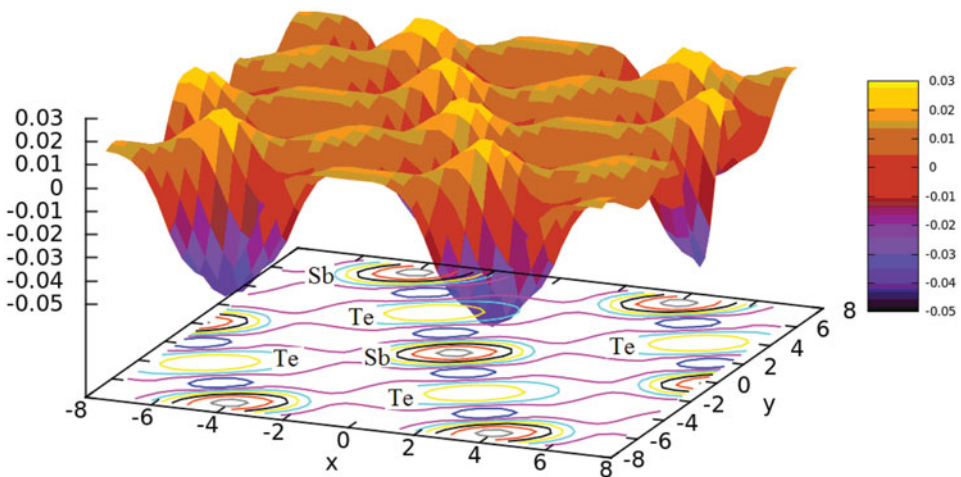
The overall shape of the charge distributions suggests covalent bonding of Sb-Te and Bi-Te. Ionicity is directly associated with the character of the chemical bond. It provides us a mean for explaining and classifying the properties of V-VI compounds. The ionicity character is dependent on the total valance charge density by calculating the charge distribution. We have used an empirical formula [26] to obtain an estimated value of the ionicity factor for  $Sb_2Te_3$  and  $Bi_2Te_3$  compounds. In this approach the ionicity parameter is defined as

$$f_i = \frac{1}{2} \left( 1 - \cos \left( \frac{E_{AS}}{E_{VB}} \right) \right)$$

Where  $E_{AS}$  is the anti-symmetry gap between the two lowest valance bands and the  $E_{VB}$  the total valance band width. The calculated value of the ionicity factor for  $Sb_2Te_3$  is 0.089 for  $E_{AS} = 1.173 \text{ eV}$  and  $E_{VB} = 13.192 \text{ eV}$ , whereas The calculated value of the ionicity factor for  $Bi_2Te_3$  is 0.089 for  $E_{AS} = 0.631 \text{ eV}$  and  $E_{VB} = 14.643 \text{ eV}$ .



**Figure 3.** The total (DOS) and projected density of states for (a)  $\text{Sb}_2\text{Te}_3$  and (b)  $\text{Bi}_2\text{Te}_3$ .



**Figure 4.** Charge density distribution of the valance charge of  $\text{Sb}_2\text{Te}_3$ .

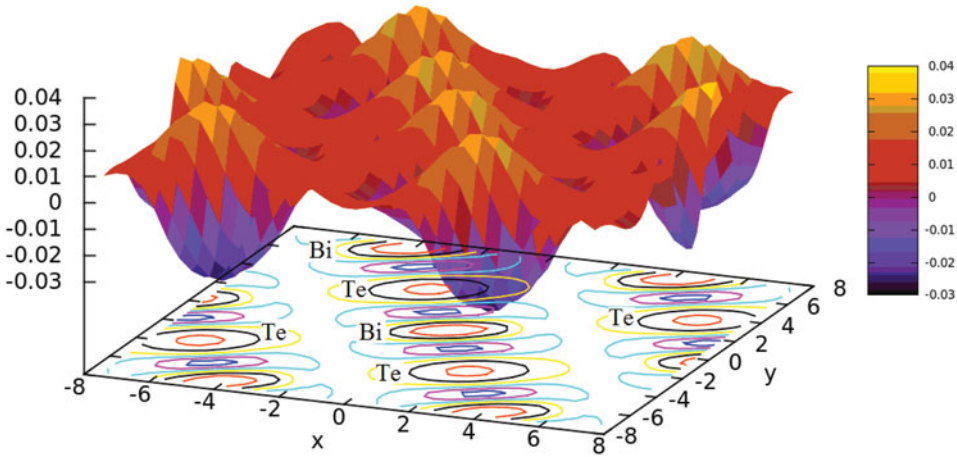


Figure 5. Charge density distribution of the valence charge of  $\text{Bi}_2\text{Te}_3$ .

### 3.3. Optical Properties

It is well known that the effect of the electric field vector,  $\mathbf{E}(\omega)$ , of the incoming light is to polarize the material. At the level of linear response, this polarization can be calculated using the following relation [27]:

$$P^i(\omega) = \chi_{ij}^{(1)}(-\omega, \omega) E^j(\omega), \quad (1)$$

where  $\chi_{ij}^{(1)}$  is the linear optical susceptibility tensor and it is given by [28]

$$\chi_{ij}^{(1)}(-\omega, \omega) = \frac{e^2}{\hbar\Omega} \sum_{nm\vec{k}} f_{nm}(\vec{k}) \frac{r_{nm}^i(\vec{k}) r_{nm}^j(\vec{k})}{\omega_{mn}(\vec{k}) - \omega} = \frac{\varepsilon_{ij}(\omega) - \delta_{ij}}{4\pi} \quad (2)$$

where  $n, m$  denote energy bands,  $f_{nm}(\vec{k}) \equiv f_m(\vec{k}) - f_n(\vec{k})$  is the Fermi occupation factor,  $\Omega$  is the normalization volume.  $\omega_{mn}(\vec{k}) \equiv \omega_m(\vec{k}) - \omega_n(\vec{k})$  are the frequency differences,  $\hbar\omega_n(\vec{k})$  is the energy of band  $n$  at wave vector  $\mathbf{k}$ . The  $r_{nm}^i$  are the matrix elements of the position operator [28].

As can be seen from Eq. (2), the dielectric function  $\varepsilon_{ij}(\omega) = 1 + 4\pi\chi_{ij}^{(1)}(-\omega, \omega)$  and the imaginary part of  $\varepsilon_{ij}(\omega)$ ,  $\varepsilon_2^{ij}(\omega)$ , is given by

$$\varepsilon_2^{ij}(\omega) = \frac{e^2}{\hbar\pi} \sum_{nm} \int d\vec{k} f_{nm}(\vec{k}) \frac{v_{nm}^i(\vec{k}) v_{nm}^j(\vec{k})}{\omega_{mn}^2} \delta(\omega - \omega_{mn}(\vec{k})). \quad (3)$$

The real part of  $\varepsilon_{ij}(\omega)$ ,  $\varepsilon_1^{ij}(\omega)$ , can be obtained by using the Kramers-Kronig transformation [28]. Because the Kohn-Sham equations determine the ground state properties, the unoccupied conduction bands as calculated have no physical significance. If they are used as single-particle states in a calculation of optical properties for semiconductors, a band gap problem comes into included in calculations of response. In order to take into account self-energy effects, in the present work, we used the ‘scissors approximation’ [27].

The known sum rules [29] can be used to determine some quantitative parameters, particularly the effective number of the valence electrons per unit cell  $N_{eff}$ , as well as the



effective optical dielectric constant  $\varepsilon_{eff}$ , which make a contribution to the optical constants of a crystal at the energy  $E_0$ . One can obtain an estimate of the distribution of oscillator strengths for both intraband and interband transitions by computing the  $N_{eff}(E_0)$  defined according to

$$N_{eff}(E) = \frac{2m\varepsilon_0}{\pi\hbar^2 e^2 N_a} \int_0^\infty \varepsilon_2(E) E dE, \quad (4)$$

Where  $N_a$  is the density of atoms in a crystal,  $e$  and  $m$  are the charge and mass of the electron, respectively and  $N_{eff}(E_0)$  is the effective number of electrons contributing to optical transitions below an energy of  $E_0$ .

Further information on the role of the core and semi-core bands may be obtained by computing the contribution which the various bands make to the static dielectric constant,  $\varepsilon_0$ . According to the Kramers-Kronig relations, one has

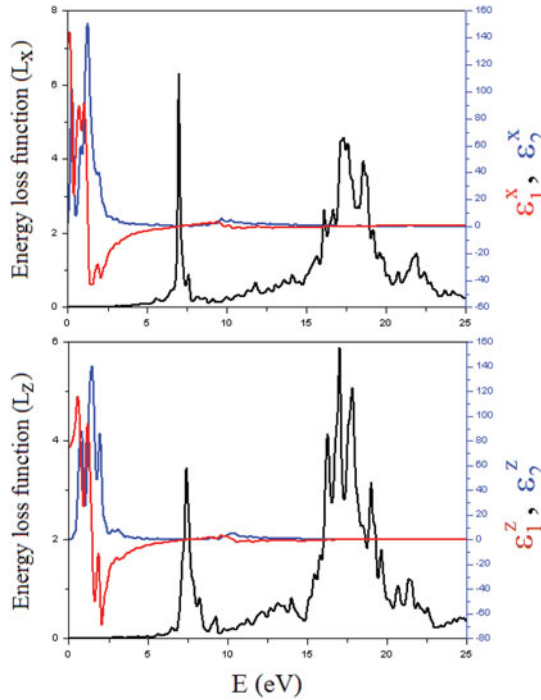
$$\varepsilon_0(E) - 1 = \frac{2}{\pi} \int_0^\infty \varepsilon_2(E) E^{-1} dE. \quad (5)$$

One can therefore define an ‘effective’ dielectric constant, which represents a different mean of the interband transitions from that represented by the sum rule, Eq. (5), according to the relation

$$\varepsilon_{eff}(E) - 1 = \frac{2}{\pi} \int_0^{E_0} \varepsilon_2(E) E^{-1} dE. \quad (6)$$

The physical meaning of  $\varepsilon_{eff}$  is quite clear:  $\varepsilon_{eff}$  is the effective optical dielectric constant governed by the interband transitions in the energy range from zero to  $E_0$ , i.e. by the polarization of the electron shells.

The  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  single crystals have a rhombohedral structure that is optically a uniaxial system. For this reason, the linear dielectric tensor of the  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  compounds have two independent components that are the diagonal elements of the linear dielectric tensor. We first calculated the real and imaginary parts of the x- and z-components of the frequency-dependent linear dielectric function and these are shown in Fig. 6 and Fig. 7. The  $\varepsilon_1^x$  behaves mainly as a classical oscillator. It vanishes (from positive to negative) at about 1.27 eV, 6.98 eV, 10.24 eV and 17.32 eV (see Fig. 6), whereas the other function  $\varepsilon_1^z$  is equal to zero at about 1.48 eV, 7.42 eV, 10.42 eV, 17.0 eV, 17.45 eV and 17.50 eV (see Fig. 6) for  $\text{Sb}_2\text{Te}_3$  compound. The  $\varepsilon_1^x$  is equal to zero at about 1.89 eV, 6.55 eV, 7.63 eV and 17.41 eV (see Fig. 7), whereas the other function  $\varepsilon_1^z$  is equal to zero at about 2.04 eV, 6.49 eV, 7.87 eV and 17.37 eV (see Fig. 7) for  $\text{Bi}_2\text{Te}_3$  compound. The peaks of the  $\varepsilon_2^x$  and  $\varepsilon_2^z$  correspond to the optical transitions from the valence band to the conduction band and are in agreement with the previous results. The maximum peak values of  $\varepsilon_2^x$  and  $\varepsilon_2^z$  for  $\text{Sb}_2\text{Te}_3$  are around 1.24 eV and 1.46 eV, respectively, whereas the maximum values of  $\varepsilon_2^x$  and  $\varepsilon_2^z$  for  $\text{Bi}_2\text{Te}_3$  are around 1.74 eV and 1.97 eV, respectively. Spectral dependences of dielectric functions show the similar features for both materials because the electronic configurations of Sb ([Kr],  $5s^2 5p^3$ ) and Bi ([Xe],  $6s^2 6p^3$ ) are very close to each other. In general, there are various contributions to the dielectric function, but Fig. 6 and Fig. 7 show only the contribution of the electronic polarizability to the dielectric function. In

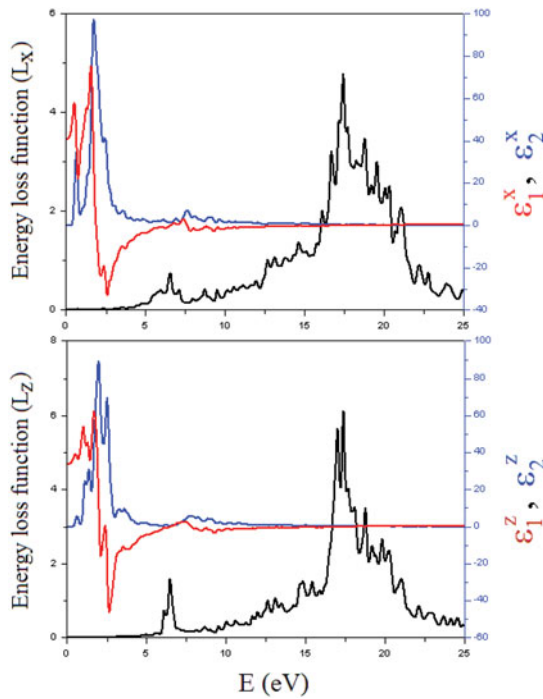


**Figure 6.** Energy spectra of dielectric function and energy-loss function ( $L$ ) along the  $x$  and  $z$  axes for  $Sb_2Te_3$  (Color figure available online).

the range between  $0.2\text{ eV}$  and  $3\text{ eV}$ ,  $\varepsilon_1^z$  decrease with increasing photon-energy, which is characteristics of an anomalous dispersion. In this energy range, the transitions between occupied and unoccupied states mainly occur between Te  $5p$  states which can be seen in the DOS displayed in Fig. 3. Furthermore as can be seen from Fig. 6 and Fig. 7, the photon-energy range up to  $0.1\text{ eV}$  is characterized by high transparency, no absorption and a small reflectivity. The  $0.1\text{--}3.0\text{ eV}$  photon energy range is characterized by strong absorption and appreciable reflectivity. The absorption band extending beyond  $7\text{ eV}$  up to  $10\text{ eV}$  is associated with the transitions from the low-lying valance subband to conduction band. Second, we see that above  $8\text{ eV}$ , corresponding to the Sb  $5s$  (Bi  $6s$ ) and Te  $5p$ . Also, we remark that the region above  $10\text{ eV}$  cannot be interpreted in term of classical oscillators. Above  $10\text{ eV}$   $\varepsilon_1$  and  $\varepsilon_2$  are dominated by linear features, increasing for  $\varepsilon_1$  and decreasing for  $\varepsilon_2$ .

The corresponding energy-loss functions,  $L(\omega)$ , are also presented in Fig. 6 and Fig. 7. In this figure,  $L_x$  and  $L_z$  correspond to the energy-loss functions along the  $x$ - and  $z$ -directions. 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 [30]. The curves of  $L_x$  and  $L_z$  in Fig. 6 and Fig. 7 have a maximum near  $17.32$  and  $17.02\text{ eV}$  for  $Sb_2Te_3$ , respectively, and  $17.42$  and  $17.38\text{ eV}$  for  $Bi_2Te_3$ , respectively.

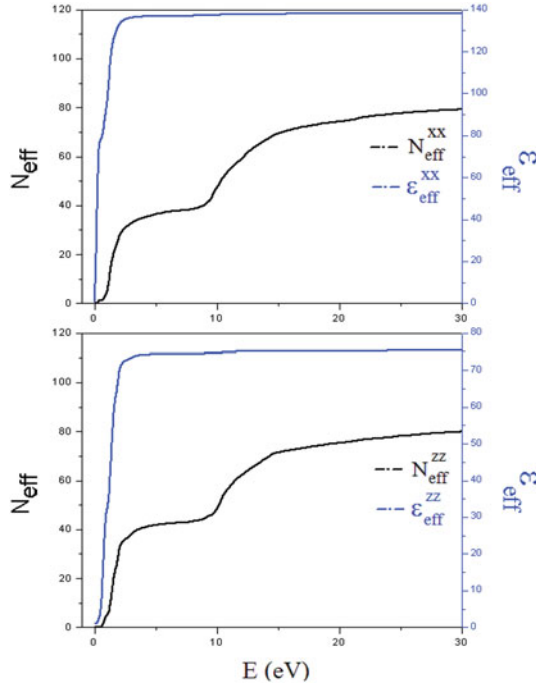
The calculated effective number of valence electrons  $N_{eff}$  and the effective dielectric constant  $\varepsilon_{eff}$  are given in Fig. 8 and Fig. 9. The effective optical dielectric constant,  $\varepsilon_{eff}$ , shown in Fig. 8 and Fig. 9, reaches a saturation value at about  $9\text{ eV}$ . The photon-energy



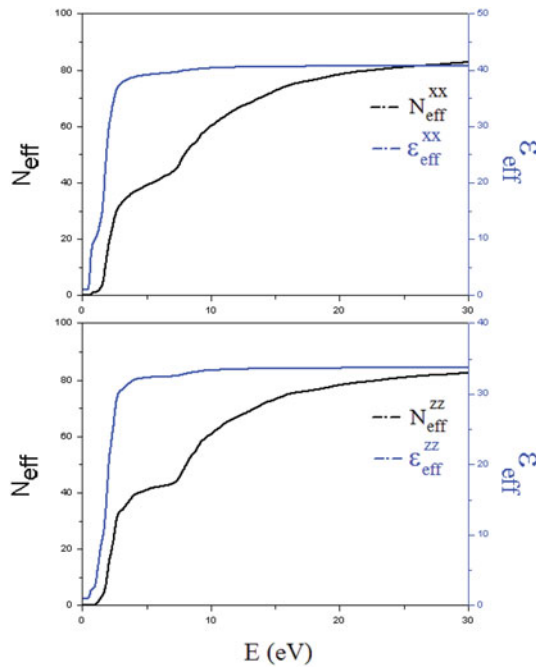
**Figure 7.** Energy spectra of dielectric function and energy-loss function ( $L$ ) along the  $x$  and  $z$  axes for  $\text{Bi}_2\text{Te}_3$  (Color figure available online).

dependence of  $\varepsilon_{eff}$  can be separated into two regions. The first is characterized by a rapid rise and it extends up to  $4\text{ eV}$ . In the second region the value of  $\varepsilon_{eff}$  rises more smoothly and slowly and tends to saturations at the energy  $9\text{ eV}$ . This means that the greatest contribution to  $\varepsilon_{eff}$  arises from interband transitions between  $0\text{ eV}$  and  $4\text{ eV}$ .

As stated above,  $N_{eff}$  (determined from the sum rule, eg. eqn (3)) is the effective number of valance electrons per unit cell at the energy  $\hbar\omega_0$  (under the condition that the entire interband transitions possible at this frequency  $\omega_0$  were made). In the case of  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  the value of  $N_{eff}$  increases with increasing photon energy and has tendency to saturate near  $9\text{ eV}$  and  $20\text{ eV}$  (see Fig. 8 and Fig. 9). Therefore, each of our plots of  $N_{eff}$  versus the photon energy for  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  can be arbitrarily divided into two parts. The first is characterized by a rapid growth of  $N_{eff}$  up to  $\sim 5\text{ eV}$  and extend to  $10\text{ eV}$ . The second part shows a smoother and slower growth of  $N_{eff}$  and tends to saturate at energies above  $30\text{ eV}$ . It is therefore so difficult to choose independent criteria for the estimate of the of valance electrons per unit cell. Recognizing that the two valance sub-bands are separated from each other and are also separated from the low-lying states of the valance band, we can assume a tendency to saturation at energies such that the transition from the corresponding sub-bands are exhausted. In other words, since  $N_{eff}$  is determined only by the behavior of  $\varepsilon_2$  and is the total oscillator strengths, the sections of the  $N_{eff}$  curves with the maximum slope, which correspond to the maxima  $dN_{eff}/d\hbar\omega$ , can be used to discern the appearance of new absorption mechanism with increasing energy ( $E = 3.8\text{ eV}$ ,  $9.5\text{ eV}$  for  $\text{Sb}_2\text{Te}_3$  and  $E = 4.2\text{ eV}$ ,  $9\text{ eV}$  for  $\text{Bi}_2\text{Te}_3$ ). The values and behavior of  $N_{eff}$  and  $\varepsilon_{eff}$  for both directions are very close to each other.



**Figure 8.** Energy spectra of  $N_{eff}$  and  $\epsilon_{eff}$  along the x and z axes for  $Sb_2Te_3$ .



**Figure 9.** Energy spectra of  $N_{eff}$  and  $\epsilon_{eff}$  along the x and z axes for  $Bi_2Te_3$ .

## Conclusion

In the present work, we have made a detailed investigation of the structural, electronic, and frequency-dependent linear optical properties of the  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  crystals using the density functional methods. The results of the structural optimization implemented using the LDA are in good agreement with the experimental and theoretical results. We have examined photon-energy dependent dielectric functions, some optical properties such as the energy-loss function, the effective number of valance electrons and the effective optical dielectric constant along the x- and z- axes.

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