

# Study of density of states and energy band structure in $\text{Bi}_2\text{Te}_3$ by using FP-LAPW method

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**Abstract.** The electronic structures for  $\text{Bi}_2\text{Te}_3$  have been investigated by first principles full potential-linearized augmented plane wave (FP-LAPW) method with Generalized Gradient Approximation (GGA). The calculated density of states (DOS) and band structure show semiconducting behavior of  $\text{Bi}_2\text{Te}_3$  with a narrow direct energy band gap of 0.3 eV.

Keywords: DFT, FP-LAPW, DOS, energy band structure, energy band gap.

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## 1. INTRODUCTION

In recent years the scientific research among the narrow band gap semiconductors are the latest trend due to their applicability in various technological sectors. Bismuth telluride ( $\text{Bi}_2\text{Te}_3$ ), a semiconductor with narrow energy band gap, is a unique multifunctional material. Semiconductors can be grown with various compositions from monoatomic layer to nano-scale islands, rows, arrays, in the art of quantum technologies and the numbers of conceivable new electronic devices are manufactured [1].  $\text{Bi}_2\text{Te}_3$  is a classic room temperature thermoelectric material[2], and it is the chalcogenide of poor metal having important technological applications in optoelectronic nano devices [3], field-emission electronic devices [4], photo-detectors and photo-electronic devices [5] and photovoltaic converters, thermoelectric cooling technologies based on the Peltier effect [6,7].  $\text{Bi}_2\text{Te}_3$  crystallizes in hexagonal crystal structure at room temperature with x, y and z- positions of atoms [8,9] as given in Table:1 and space group is 166 R-3m . The hexagonal crystal structure of  $\text{Bi}_2\text{Te}_3$  is illustrated in Fig.1. In this report, we would like to present a systematic study of DOS and energy band structures of  $\text{Bi}_2\text{Te}_3$  using FP-LAPW method.

**Table : 1**

| Atom | X           | Y           | Z           |
|------|-------------|-------------|-------------|
| Bi   | $\pm 0.4$   | $\pm 0.4$   | $\pm 0.4$   |
| Te 1 | 0           | 0           | 0           |
| Te 2 | $\pm 0.212$ | $\pm 0.212$ | $\pm 0.212$ |

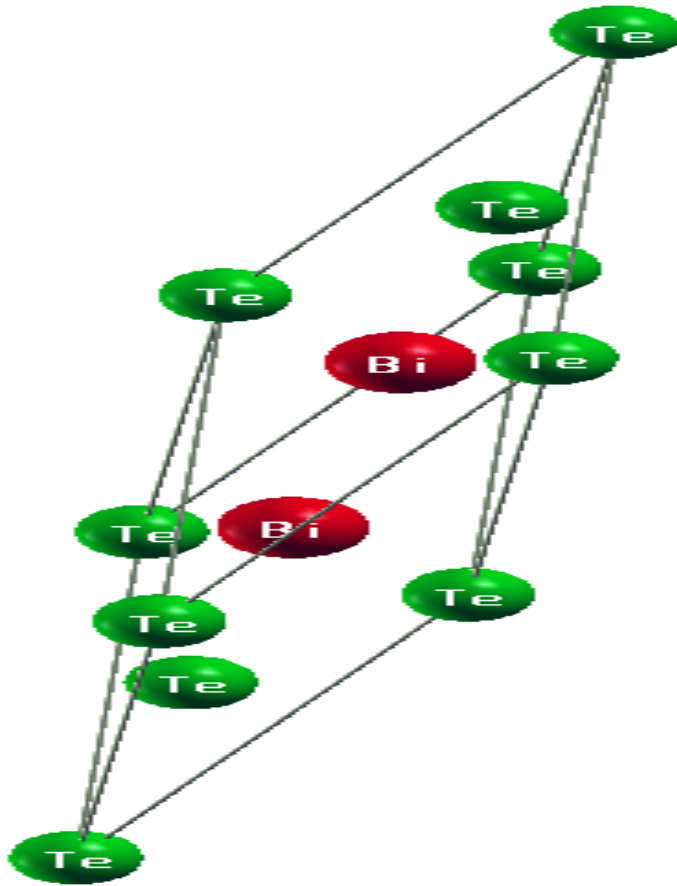


Fig.1 : Unit cell structure of  $\text{Bi}_2\text{Te}_3$

## 2. THEORY AND COMPUTATIONAL METHODS

First principles FP-LAPW [10] method based on density functional theory ( DFT ) is used for calculations of DOS and band structure of  $\text{Bi}_2\text{Te}_3$ . The calculated total energy (E) within GGA[11] as a function of the volume (V) were used for determination of theoretical lattice constants. Equilibrium lattice constants are calculated by fitting the calculated total energy to the Murnaghan's equation of state [12]. A series of total energy calculations as a function of volume can be fitted to an equation of states according to Murnaghan.

$$E(V) = E_0 + \frac{(V_0)^{B'_0}}{B'_0 - 1} + \frac{B_0 V_0}{B'_0 - 1} \quad (1)$$

where  $E_0$  is the minimum energy at  $T = 0\text{K}$ ,  $B_0$  is the bulk modulus at the equilibrium volume and  $B'_0$  is pressure derivative of the bulk modulus at the equilibrium volume. The equilibrium volume is given by the corresponding total energy minimum as shown in Fig.2 [13]. The equilibrium lattice constant was optimized using the experimental values of  $a= 4.383$ ,  $b=4.383$  and  $c= 30.487 \text{ \AA}$  [8,9]. The calculation was accomplished by using the WIEN2K code [14]. For exchange-correlation, we have used GGA. In the FP-LAPW procedure, wave functions, charge density and potential are expanded in spherical harmonics within non overlapping atomic spheres of radius  $R_{\text{mt}}$  and in the

remaining space of the unit cell plane waves are considered. The maximum multi-polarity  $l$  for the waves inside the atomic spheres was confined within  $l_{\max} = 10$ . The wave functions in the interstitial region were expanded in plane waves with a cut-off of to  $K_{\max} = 2.5 \text{ a.u.}^{-1}$  (where  $K_{\max}$  is the maximum value of the wave vector  $\mathbf{K} = \mathbf{k} + \mathbf{G}$ ). For Bi:  $6s$ ,  $6p$  and Te:  $5s$ ,  $5p$  states were treated as valance state and all other lower states were treated as core state. The potential and charge density were expanded upto a cut-off  $G_{\max} = 12 \text{ a.u.}^{-1}$ . The muffin-tin radii are set to  $R_{\text{mt}} = 2.5 \text{ a.u.}$  for Bi and  $2.5 \text{ a.u.}$  for Te in  $\text{Bi}_2\text{Te}_3$ . A mesh of 2000 k-points was used after doing k- optimization. The calculated lattice constants found by volume optimization are  $a = 3.329 \text{ \AA}$ ,  $b = 3.329 \text{ \AA}$  and  $c = 17.190 \text{ \AA}$  for  $\text{Bi}_2\text{Te}_3$  which are shown in Fig.2.

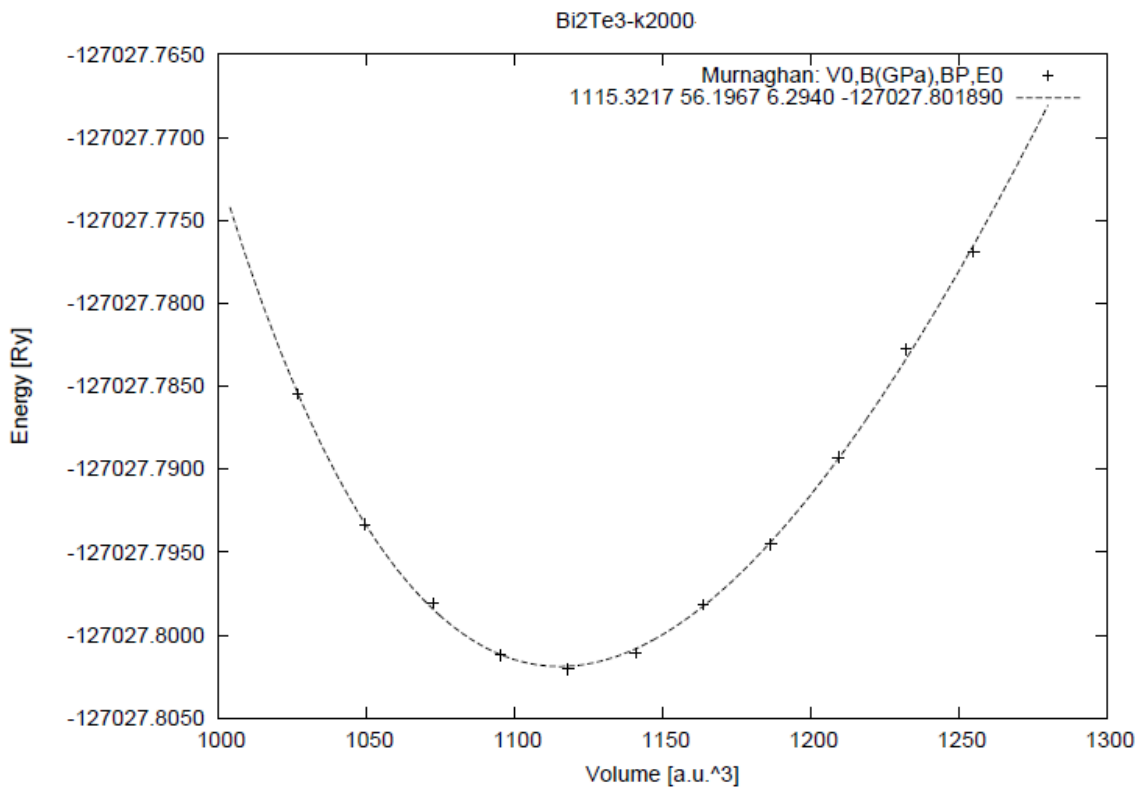


Fig.

2: Energy versus Volume curve using the volume optimization method for  $\text{Bi}_2\text{Te}_3$

### 3. RESULTS AND DISCUSSIONS

The total and partial DOS plots of  $\text{Bi}_2\text{Te}_3$  are shown in Figs.3,4 & 5. From Fig.3, we found that the contributions to total DOS were from Bi- $6p$  and Te- $5p$  electron states. The core region which is below  $-6\text{eV}$  is formed by  $6s$  electron state of Bi and a sharp peak at around  $-11 \text{ eV}$  is observed [Fig.4]. The conduction region, which is above the Fermi level, is mainly contributed by Bi- $6p$  and Te- $5p$  state electrons [Figs.4 & 5]. In the valence region (below Fermi level), we have observed, Bi- $6p$  and Te- $5p$  electron states are mainly contributing to total DOS giving a sharp peak at around  $-1.0\text{eV}$  [Fig.5].

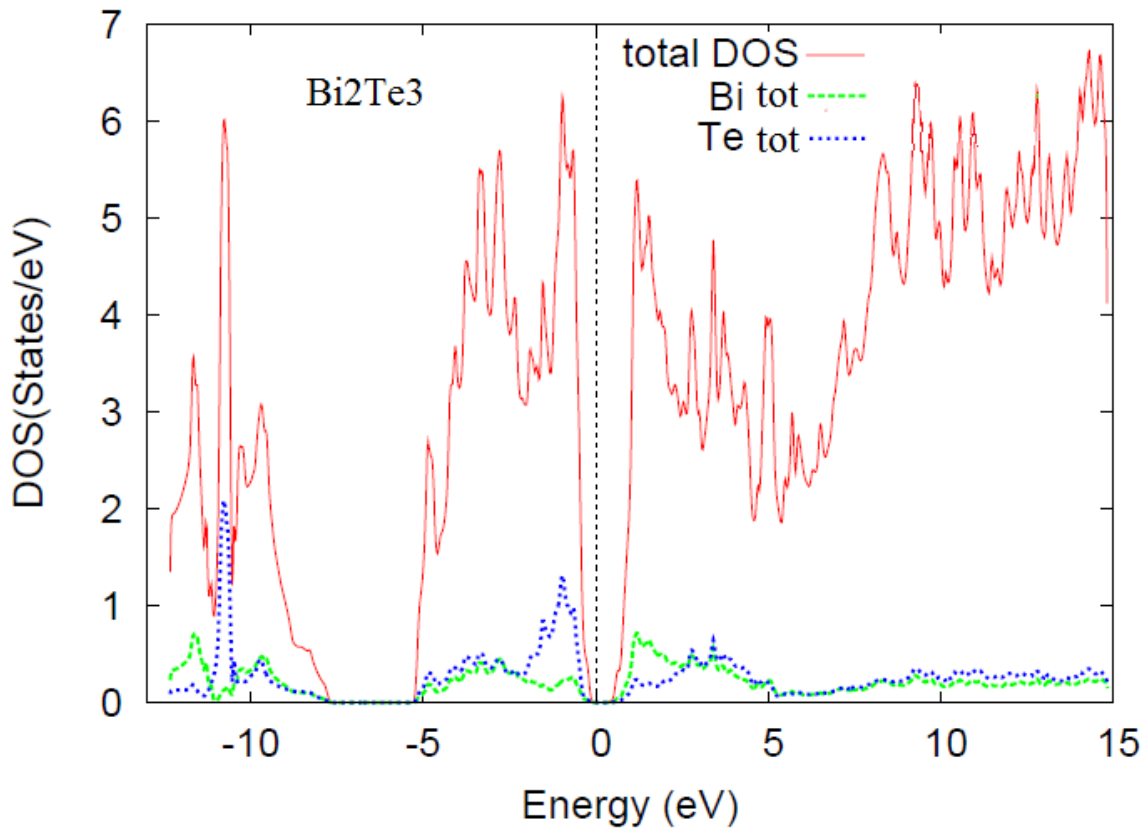


Fig. 3: Bi<sub>2</sub>Te<sub>3</sub>-total, Bi-Total and Te-total (Energy= 0 eV corresponds to Fermi level, E<sub>F</sub>)

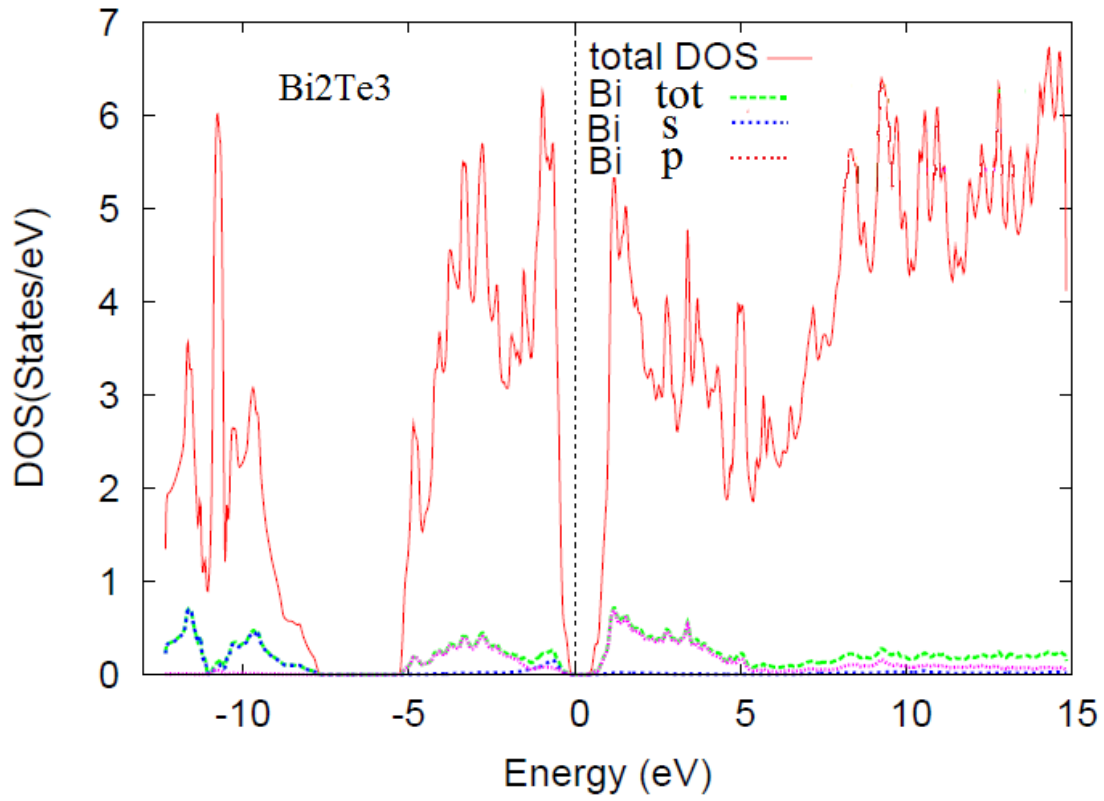


Fig. 4 : total DOS, Bi-total, Bi-s & Bi-p states of Bi<sub>2</sub>Te<sub>3</sub>

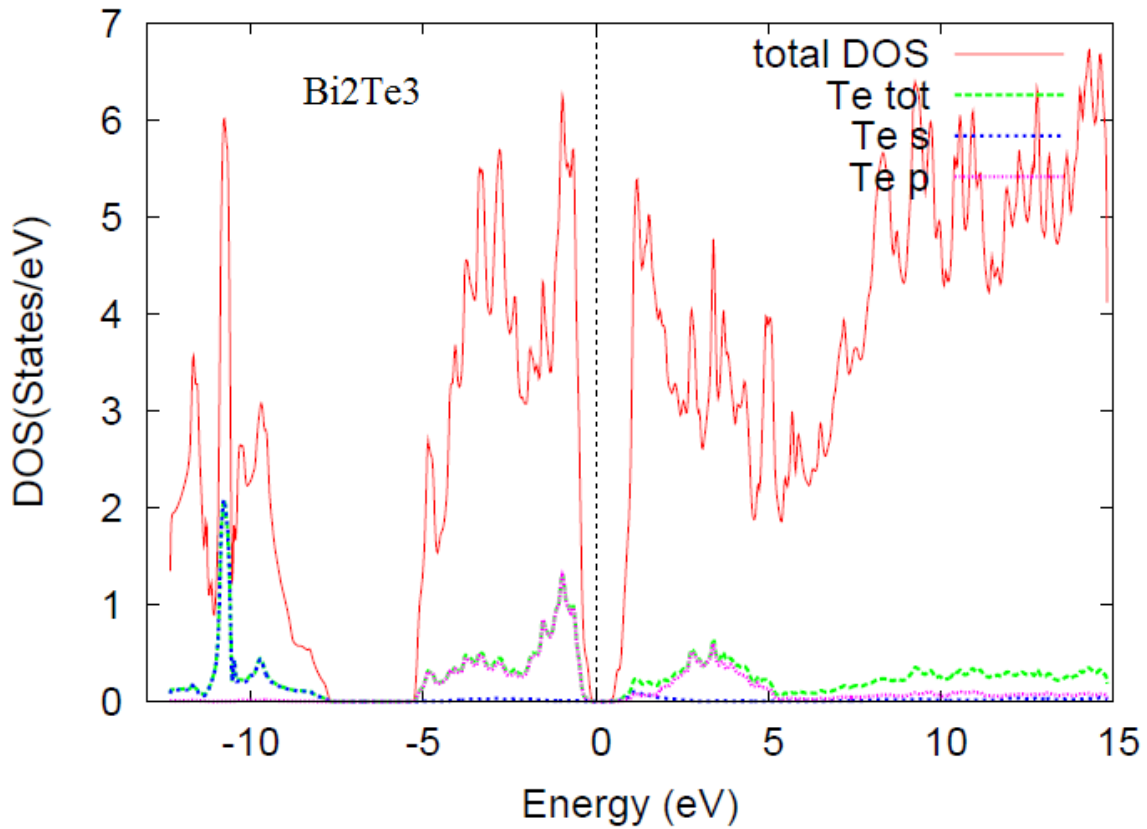


Fig.5: total DOS, Te-total, Te-s, Te-p states of  $\text{Bi}_2\text{Te}_3$

From the band structure plot [Fig.6] we observed a direct band gap of the order of 0.3 eV occurring at symmetry point  $\Gamma$ . The band structure plot was also found with higher number of bands at the regions where peaks of the DOS were observed. In Fig.7, we have compared band structure with DOS plot of  $\text{Bi}_2\text{Te}_3$  and found that higher DOS regions correspond to more bands.

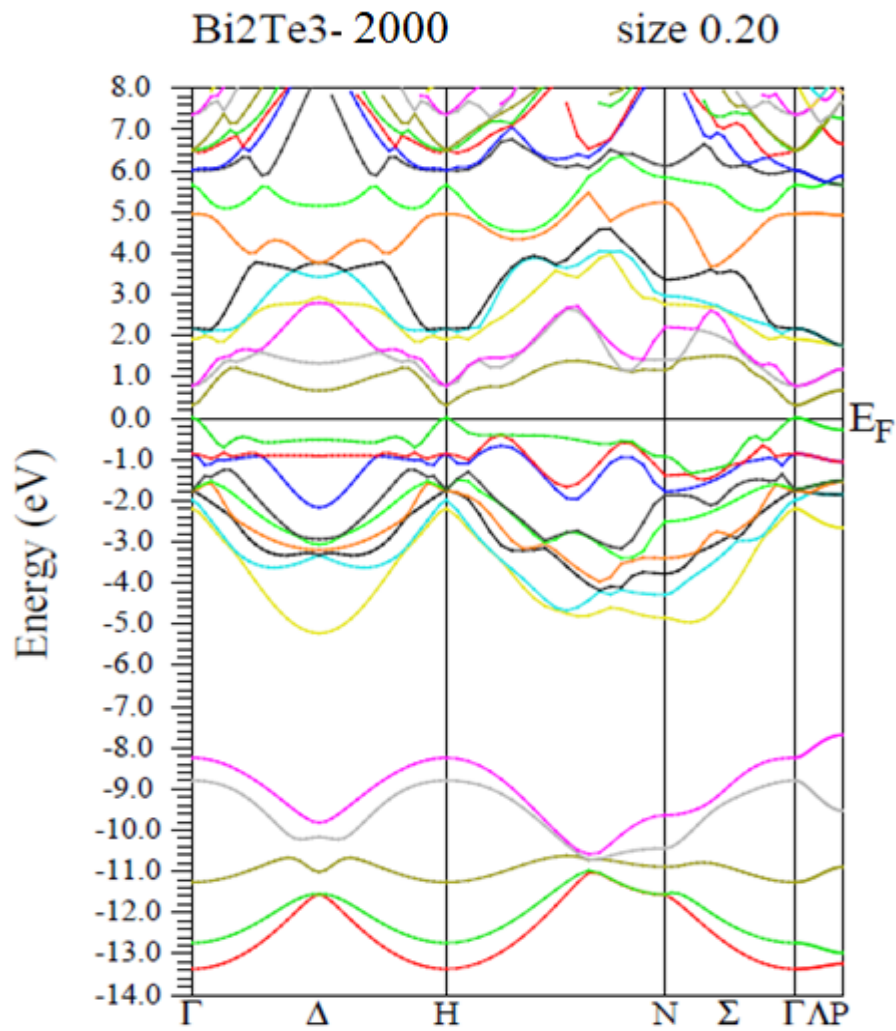


Fig.6: The plot of band structure of Bi<sub>2</sub>Te<sub>3</sub>.

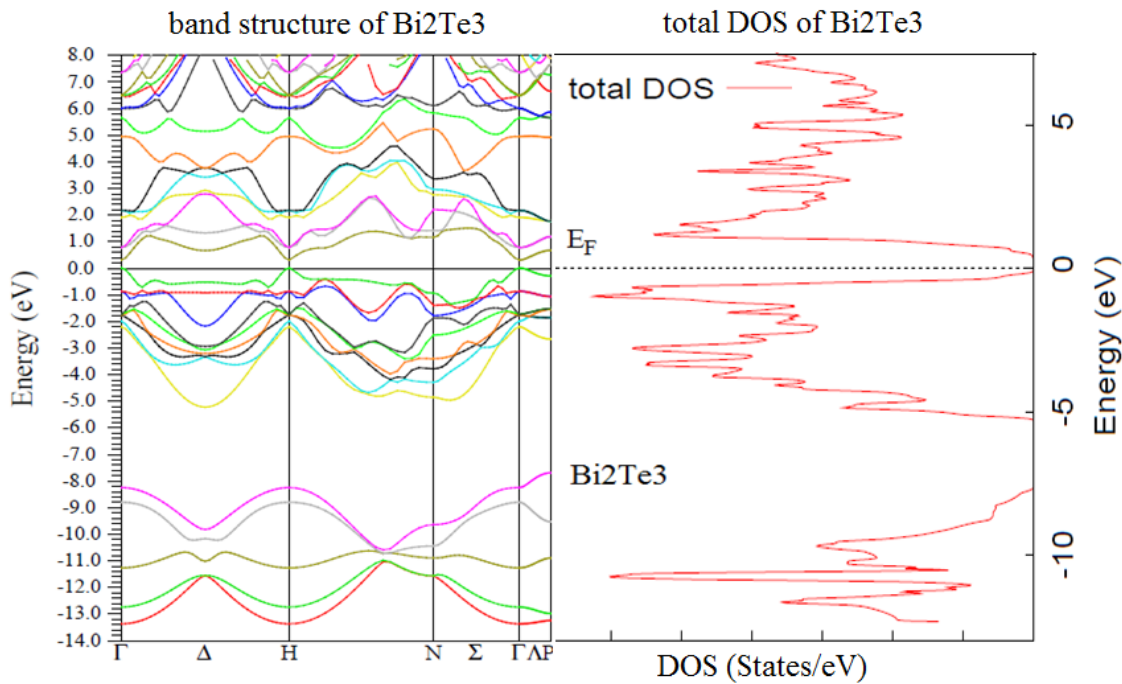


Fig.7:

Band structure combined with DOS plot of  $\text{Bi}_2\text{Te}_3$   
 (Energy=0eV corresponds to Fermi Level,  $E_F$ )

#### 4. CONCLUSIONS

In conclusion, we have observed a qualitative agreement between theoretical and experimental lattice constants[8,9]. Calculated band gap is close to experimental value. Band gap of the order of 0.3 eV suggests that  $\text{Bi}_2\text{Te}_3$  is a semiconductor with small energy gap. The presence of narrow band and the dense band energies near Fermi Energy suggests that the compound can be used as suitable candidate for thermoelectric applications. However, we have found that the calculated band gap in our case deviated from the previous results which may account for the insufficiency in our approximation which failed to treat the semicore states more accurately. Moreover the GGA band gap, is underestimated as compared to the experimental one, that is 0.14 eV[15], as usual. This discrepancy might be solved by using some other appropriate approximation like mBJ [16] which treats the core and semicore states more efficiently, to mimic the experimental results accurately. We intend to check this discrepancy by inclusion of mBJ potential[16] which had been done by Amit *et al* [17].

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