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FIRST PRINCIPLE CALCULATION OF ELECTRONIC STRUCTURE, DENSITY OF STATE AND DIELECTRIC FUNCTION OF BISMUTH TELLURIUM IODINE

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Abstract. The electronic structure, total and partial density of states (DOS) and dielectric functions of BiTeI are calculated by using full potential-linearized augmented plane wave (FP-LAPW) method in the framework density functional theory (DFT) with the generalized gradient approximation (GGA) by WIEN2k package. Our calculations show that BiTeI is a narrow band gap semiconductor with taking into account spin splitting at the band edges. In the presented article the relevant interband optical transitions are found and given the interpretation within a calculated band structure.

Keywords: *first principle, optical transition, electronic structure, dielectric function, the density of state.*

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1. Introduction

BiTeI due to the emergence of giant Rashba-type spin splittings in its band structure has a great deal of interest as a potential spintronic material (Ishizaka *et al*., 2011). Making use of these effects to control the electron spin is a central goal in spintronics. The ability to use effects such as the generation of topologically protected states with the influence of spin-orbit interaction on the electronic wave functions whereby electron spin can be controlled is the main goal in spintronics. Crystals with the layered structure are investigated widely due to their extraordinary bulk, surface electronic properties which are useful for various technological applications (Butler *et al*., 2013; Crepaldi *et al*., 2014). Using heavy atoms (Bi2Te3 and Bi2Se3) which realize topological insulators with nontrivial spin-polarized surface states, can achieve strong spin-orbit effects (Hasan & Kene, 2010).

The crystal structure of BiTeI is the hexagonal type and Bi, Te, I atoms occupy the 1*a*, 1*c*, and 1*b* positions with fractional coordinates (0,0,0), (2/3,1/3,*z*Te), and (1/3,2/3,*z*I), respectively. In Kulbachinski et al. (2012) the electronic structures were calculated for BiTeI using the density-functional theory approach and accounting for the strong spin-orbital interaction. The band structures of the compound, showing strong mixing of the p states of all elements in the vicinity of the Fermi level, with the band gap of 0.478 eV.

Sobolev et al. (2004) is reported the result of the dielectric permittivity and volume electron energy loss spectra of the ferroelectric semiconductor BiTeI for the E ⊥ c polarization in the range 0–12 eV. Their result shows six maxima at 2.12, 2.66, 3.21, 4.39, 7.89, and 9.84 eV in the ε2(E) spectrum.

Taking into account that the detailed information about the optical properties of a compound is provided by spectra of more than ten optical characteristics (the reflection coefficient (R), imaginary (ε2) and real (ε1) parts of dielectric permittivity (ε), imaginary (Im) and real (Re) parts of the volume electron energy loss function, and others Sobolev & Nemoshkalenko, (1988)) this work devoted to calculation of dielectric function, electronic structure, total and partial density of state of compound.

2. Computational Details

In this work, the DFT-based full-potential linearized augmented plane wave (FP-LAPW) method utilized in the Wien2K code (Blaha *et al*., 2008) was used to study the physical properties of the BiTeI compound. As exchange-correlation potential the GGA suggested by Perdew et al. (1996) was used. Suitable sphere radius (RMT) for the Bi, Te, I atomsare selected together with a mesh of 1000 k-points in the full Brillouin zone (BZ). Inside the spherical MT region, the wave function is expanded by spherical harmonics up tolmax= 10.0. The cut-off energy for separation of the core and valence states was set to -8.5 Ry. Self-consistency is achieved with an energy convergence of 10^{-5}eV. The influence of relativistic effects on the electronic properties is taken into account with scalar relativistic approximation. The imaginary part of dielectric function in the range of optical frequencies was obtained by calculating the joint density-of-states for optical transitions between the valence and conduction bands, using the Monchorst-Pack technique for integration over the BZ. The real part was obtained from the imaginary part by Kramers-Kronig transformation.

3. Result and discussion

Our electronic band structures calculation along the high-symmetry lines of the BZ without taking into account Spin-orbit coupling (SOC) reveals that BiTeIis a semiconductor, with band gap energy 1.23eV Fig. 1a. Taking into account the SOC, the maximum of the valence band and the minimum of the conduction band are moved to each other which leads to decreasing of energy gap and becomes 0.24eV (Fig. 1b).

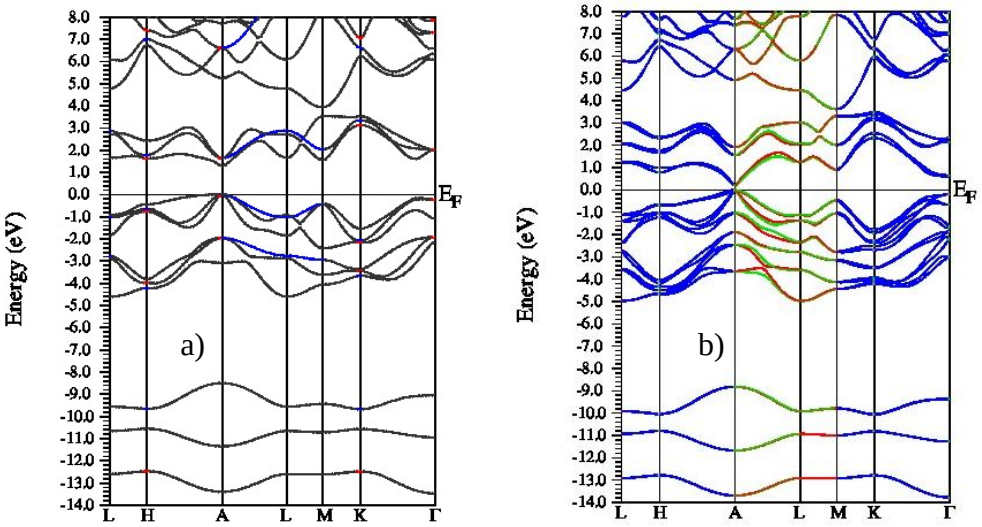

Fig.1. Calculated electronic structure without SOC (a) and with SOC (b)

This result is in good agreement with experimental data (Sakano *et al*., 2012) where Eg= 0.26eV and with calculated by *ab initio* simulation package(VASP) Eg=0.21eV (Guler-Kilic & Kilic, 2015). The total density of states (DOS) and partial densities of states (PDOS) allow determining bonding nature, hybridization of states and contribution of orbitals to the band structure of materials.

In Fig.2.have been shown total DOS and PDOS of Bi, Te and I atoms in BiTeI calculated with SOC. From the PDOS calculation (Figure 2) the lowest valence bands at the bottom (-12 to -13 eV) are due to 6s and 5s states of Bi and Te atoms respectively. The major contribution to the valence band group in -5 ÷ -3 eV is from the 4s states of I atoms and the 6s states of Bi atoms. The valence states, from -2 eV up to the Fermi energy, is dominated by the Te-5p states with a small component from the I-3p states. The bottom of the conduction band basically originates from 6p states of Bi atoms and partially from Te-5p states. Energy peak around 3 eV to 4 eV is a contribution from the Bi-6p and Te-5p states.

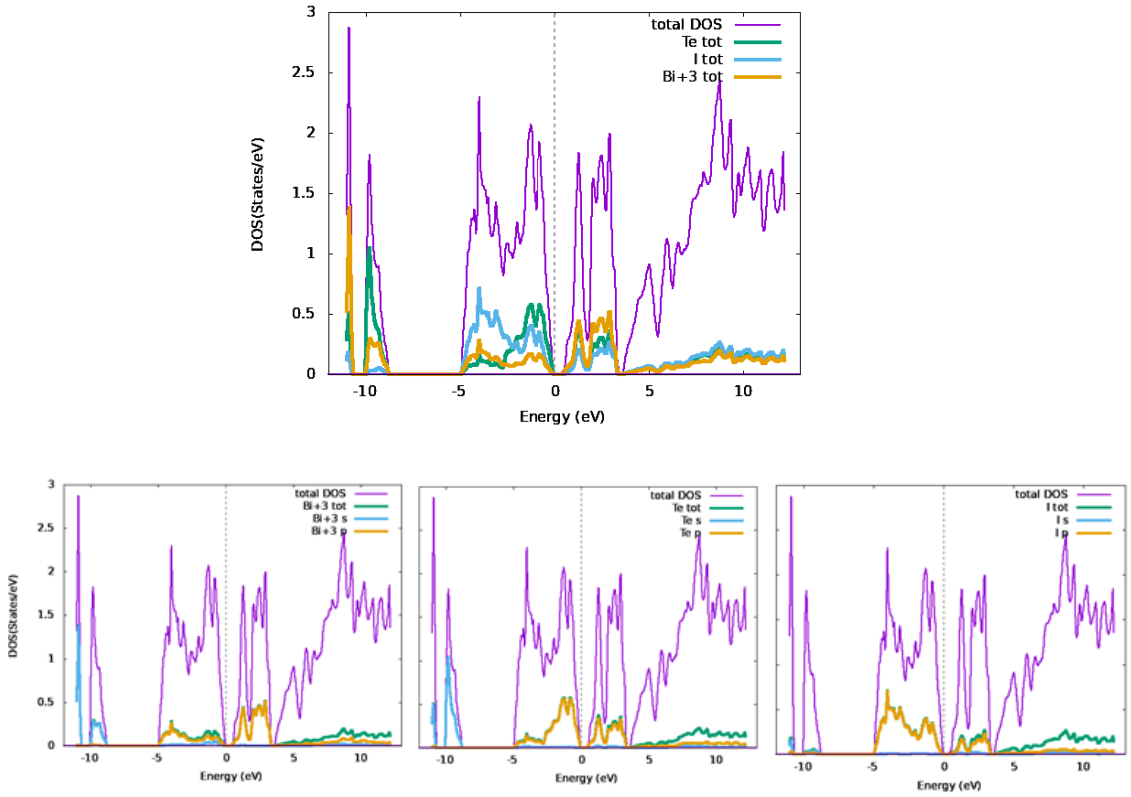

Fig.2. Calculated total and partial density of state

The calculated optical functions at the optimized crystal structure are presented in Fig.3 for the energy range up to 8 eV along with two principal directions for crystals of hexagonal symmetry the x-, and z-direction, $\varepsilon_{\perp}$, and $\varepsilon_{||}$, respectively.

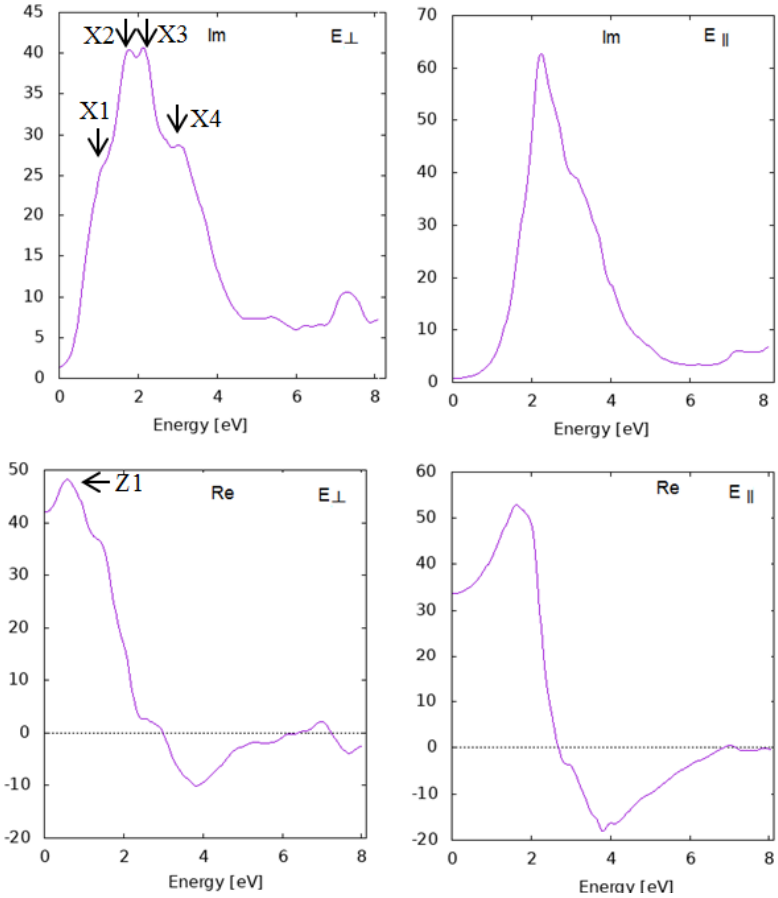

Fig.3. Calculated the real and imaginary part of dielectric functions

From the relevant interband optical transitions are found that the highest peak X2 and X3 for $\varepsilon_{\perp}$and Z1 for $\varepsilon_{\parallel}$ polarization localized at about 1.8 and 2.1 eV(X1 and X2) and 1.02eV respectively can be mainly assigned to the electronic interband transitions between Te5p→Bi6p states. Calculation result shows that s state of Bi, Te and I is not significant for optical transitions.

4. Conclusion

We have made a detailed investigation of the electronic structure, band structure and DOS of BiTeI using the FP-LAPW method. The electronic structure obtained from first-principles calculations are compared with experimental results. From total and partial DOS it has been concluded that the top of the valence band is mainly from Te-5p states with a small component from the I-3p states and the lower part of the conduction band is formed by bonding states between the Bi- 6p and Te - 5p orbitals. From the relevant interband optical transitions are found that the highest peak X2 and X3 for $\varepsilon_{\perp}$and Z1 for $\varepsilon_{\parallel}$ polarization localized at about 1.8 and 2.1 eV(X1 and X2) and 1.02eV respectively can be mainly assigned to the electronic interband transitions between Te5p→Bi6p states.

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