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FULL PAPER

Density functional theory study of electronic properties of Bi_2Se_3 and Bi_2Te_3

Abdullahi Lawal [a,b,*], Amiruddin Shaari [a]

[a] Department of Physics, Faculty of Science, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia
[b] Department of Physics, School of Science, Federal Collage of Education, Zaria, Kaduna State, Nigeria

* Corresponding author: abdullahikubau@yahoo.com

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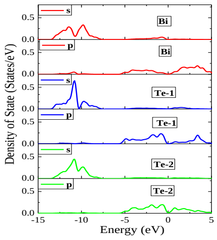
Graphical abstract



Abstract

Bi_2Se_3 and Bi_2Te_3 topological insulators are layered narrow gap semiconductors materials with hexagonal unit cell similar to graphene. The conducting states on their surface or edge are exciting features for future optoelectronic application. In this paper, we present here ab initio study of electronics properties of Bi_2Se_3 and Bi_2Te_3 compound without and with spin-orbit interaction using first-principles approach. Structural, band structure, total density of state (DOS), partial density of state (PDOS) were determined by Quantum-Espresso simulation package which uses plane wave basis and pseudopotential for the core electrons, while treating exchange-correlation potential with generalized gradient approximation (GGA). From our computations, the obtained results were found to be consistent with the available experimental results.

Keywords: Topological insulator, quantum-espresso, DFT

INTRODUCTION

Topological insulators are new class of narrow band gap semiconducting materials characterized by the presence of strong spin orbit (SO) interactions, which invert the orbital character of conduction and valence bands [1-4]. In topological insulators, there exist surface states at all energies with a linear dispersion with respect to the surface momentum k, and the spin polarization varies with k [1]. The main potential applications of TIs based devices: quantum computing, spintronics, enhanced thermoelectric effects, optical recording, high performance field effect transistor, laser photonics and high speed optoelectronics etc [2, 5-7]. Recently, Bi_2Te_3 and Bi_2Se_3 Tis have been studied for their special electronic properties, namely, the formation of a single Dirac cone inside the bulk band gap by the surface state leading to tuneable surface band gap which is a key requirement of many optoelectronic devices [5, 8]. In order to better understand the optoelectronic properties of topological insulators such as strong light absorption, photocurrent sensitivity to the polarization of light it is essential to determine it electronic properties. Topological insulators, mainly Bi_2Te_3 and Bi_2Se_3 compound are narrow band gap semiconductor material which because of their electronic and optical properties plays an important role in broadband optoelectronic devices; these semiconductors have one of the highest figures of merit at room temperature [9]. Theoretical investigation by various ab-initio methods and experimental studies has shown that Bi_2Te_3 and Bi_2Se_3 is a narrow-gap semiconductor and the gap structure strongly depends on spin-orbit coupling [10].

The rhombohedral crystal structure of Bi_2Se_3 and Bi_2Te_3 contain five atoms per unit cell with three Te (Se) atoms differentiated by two atoms as Te1 (Se1) and the other as Te2 (Se2) which belong to (R-3m) space group while the Bi atoms are equivalent. Alternatively three rhombohedral unit cells of Bi_2Se_3 and Bi_2Te_3 structure form hexagonal unit cell containing 15 atoms with layered structure regards as quintuple layered inform of a slab of five atomic layers shown in Fig.1b [9, 11]. Quintuple layers held together along vertical axis by a very weak van der Waals bonding between neighbouring QLs [1, 12].

Most of the electronic structure calculations for Bi_2Se_3 and $Bi_2Te_3$are performed with experimental data without full relaxation. In this paper, we explore the calculation of band structure, density of state (DOS) and partial density of state of state (PDOS) of Bi_2Te_3 and Bi_2Se_3 with full relaxation. Based on these optimized reference structure, we find that the band gap is in excellent agreement with the experimental results.

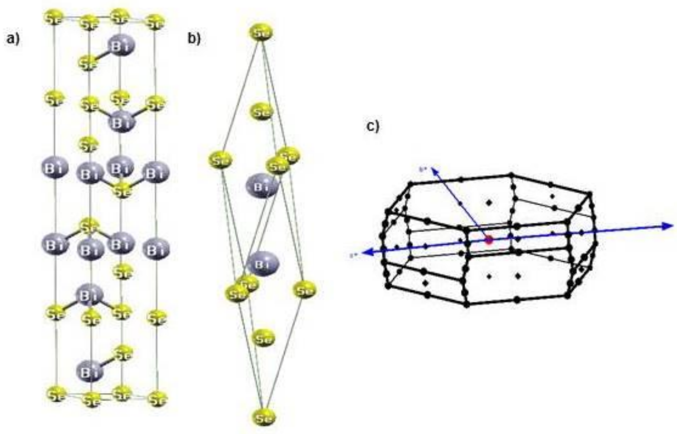


Fig. 1 Structure of bulk Bi_2Se_3 (a) Rhombohedral unit cell. (b) Hexagonal unit cells (c) Bulk primitive Brilliound zone of Bi_2Se_3 and Bi_2Te_3

COMPUTATIONAL METHODS

The band structure and density of states were calculated by pseudopotential and plane-wave basis set method within the density functional theory (DFT),treating exchange-correlation functional with generalized gradient approximation (GGA) in the form of Perdew–Berke–Erzndof (PBE) functional [3]. All pseudopotentials used in the calculations were norm-conserving scalar relativistic and full relativistic pseudopotentials. The spin orbit coupling is included in the calculation as Bi, Se and Te atoms are heavy elements the effects were treated using fully relativistic norm-conserving pseudopotentials. All calculations were performed within the Quantum-Espresso package [4]. Plane-wave kinetic energy cut-offs were set at 55 and 82 Ry with charge density of 475 Ry for Bi_2Se_3 and Bi_2Te_3, respectively. The Brillouin zone was sampled with a 10×10×10 Monkhorst-Pack grid of k-points [4]. The geometry relaxation calculations were performed as a results of the Born Openheimer approximation, this stage involves the determination of the cell parameters and the atomic coordinates that minimize the energy function within the adopted numerical approximations using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm [4, 13, 14].

RESULTS AND DISCUSSION

The rhombohedral unit cell of Bulk Bi_2Se_3 and Bi_2Te_3 have space group of D_53^d(R-3m) as shown in fig.1 (b). The band structures calculation of Bi_2Se_3 and Bi_2Te_3 within GGA with and without taking into account the spin-orbit coupling along high-symmetry Γ→Z→F→Γ→L are plotted with Fermi level set at 0 eV on energy scale in band gap plots as shown in Fig.2 and Fig.3 in order to observe the effects of SOC on the topological properties of Bi_2Se_3 and Bi_2Te_3. Spin-orbit coupling calculations were performed with full relativistic pseudopotentials [9]. From the calculations of band structures and the total density of states, we get the value of the energy gap of Bi_2Se_3 to be around 0.33 eV, conversely for Bi_2Te_3 the band gap calculated were 0.13 eV. These values are close to the experimental one of 0.32 eV and 0.11eV [15, 16]. On the other hand, the shape of the band found in this work is almost similar to that of previous work [3, 9, 17-20].

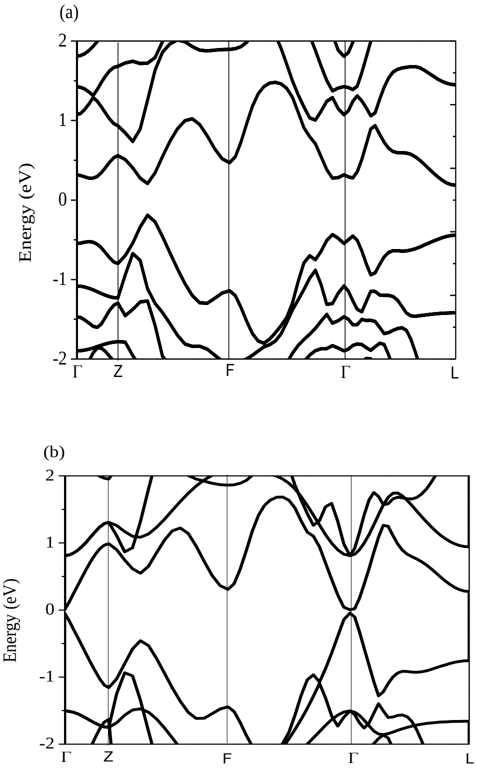


Fig. 2 Band structure of bulk Bi2Se3 with SOC and without SOC.

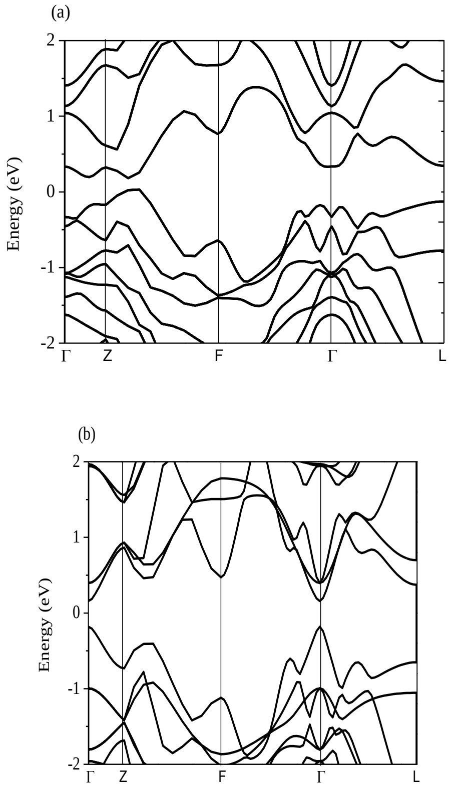


Fig.3 Band structure of bulk Bi_2Te_3 with SOC without SOC.

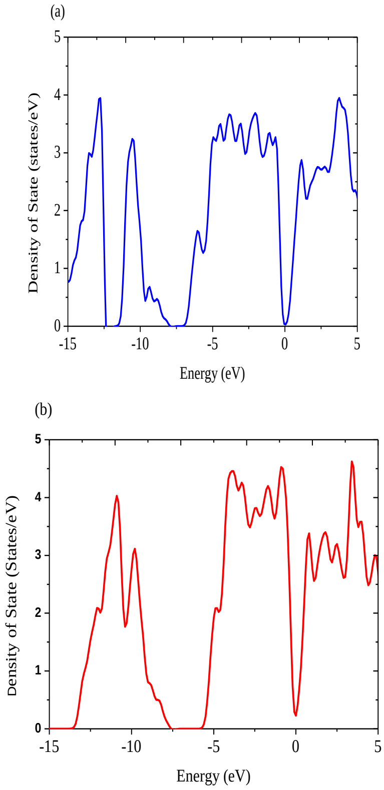


Fig.4 Density of state for (a) Bi_2Se_3 (b) Bi_2Te_3

The results of total and partial densities of states (DOS and PDOS) of Bi_2Te_3 and Bi_2Se_3 help to further elaborate the nature of band gap as shown in Fig.4 and Fig.5. The partial density of states gives information about the origin of bands, in the case of Bi_2Te_3, the s-orbital of Bi, and the s-orbital of both Te-1 and Te-2 atoms contribute the most states to the core bands while p-orbitals of Te-1 and Te-2 contribute the most states to valence bands. The p-orbitals of Bi atoms contribute the most to the conduction bands.

Table 1 Obtained results for Bi_2Te_3 and Bi_2Se_3 compounds

Physical properties	**Bi_2Te_3**	**Bi_2Se_3**
Present Work		
Eg (eV)-WithSOC	0.13	0.33
Eg (eV)-WithoutSOC	0.31	0.06
Other Work Theoretical Eg (eV)-WithSOC	0.12[18],0.10[4],0.154[21],0.13[4]	0.32[18],0.3[22],0.9[23],0.32[16]
Eg (eV) WithoutSOC	0.28[18],0.17[19]	0.3[11],0.04[19]
Experimental		
Eg (eV)	0.11[15],0.16[24],0.149[14]	0.32[16],0.6[14,25]

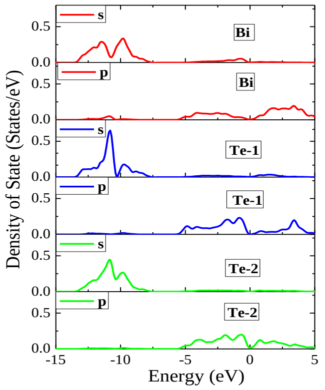


Fig. 5 Partial density of state for Bi_2Te_3

CONCLUSION

In the paper, we presented results of electronic properties of Bi_2Te_3 and Bi_2Se_3. The electronic band structure and density of state (DOS) was calculated using ab initio pseudopotential method within DFT framework implemented in the code Quantum Espresso. Our calculation clearly shows that the results with SOC are in good agreement with experimental and theoretical data in previous work. Hence, spin-orbit coupling needs to be included in calculation in order to give more accurate results.

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