# First-principles Electronic Structure Calculation of Topological Insulator $Bi_2Te_3$

**P.Taivansaikhan[1*], N.Tsogbadrakh[2**] and S.C.Hong[1]**

*[1]Department of Physics and Energy Harvest-Storage Research Center, University of Ulsan, Ulsan 680-749, Republic of Korea*
*[2]Department of Theoretical Physics, School of Physics and Electronics,*
*National University of Mongolia, University Strteet-1, Ulaanbaatar-210646, Mongolia*
**E-mail: p_taivansaikhan@yahoo.com **E-mail:Tsogbadrakh@num.edu.mn*

Bismuth telluride ($Bi_2Te_3$) attracts much attention as a topological insulator. Using the first-principles density-functional calculations based on generalized gradient approximation, the structural and electronic properties of $Bi_2Te_3$ have been done with and without spin-orbit coupling (SOC). Total energy calculations showed that the optimized lattice parameters are *a*= *b*= 4.44 Å and *c*= 32.20 Å, in consistent with an experiment. $Bi_2Te_3$ is calculated to be an insulating with band gap of 0.5 eV from the density of states without SOC. Finally, we found that the effect of SOC is a crucial to determine the experimentally observed very narrow band gap of 0.15 eV.

**Keywords:** $Bi_2Te_3$, First-principles, Spin-orbit coupling, Time reversal symmetry, Band structure, Density of states

## I.INTRODUCTION

One of the recent big issues in condensed matter physics is the discovery of topological insulators (TIs) [1]. TIs are electronic materials that have a bulk band gap like an ordinary insulator but have protected conducting states on their edge or surface. These states are possible due to the combination of the spin-orbit coupling interaction (SOC) and time-reversal symmetry (TRS) [2-5]. TIs are interesting not only because of their fundamental importance but also their great potential for future applications.

In early studies of TIs, due to the absence of realistic materials, most discussions were based on the model Hamiltonians [2-5]. However, within the last couple of years this field has been strongly motivated by the discovery of several real compounds.

In two dimensions, the topological insulator is a quantum spin Hall insulator [6,7], which is a close cousin of the integer quantum Hall state.

Recently, tetradymite semiconductors $Bi_2Te_3$, $Bi_2Se_3$, and $Sb_2Te_3$ have been theoretically predicted [8-10] and experimentally observed [11,12] to be three dimensional TIs with the bulk band gap.

## II.COMPUTATIONAL METHOD

The bulk $Bi_2Te_3$ has a rhombohedral crystal structure with space group $D_{3d}^5$ (*R*3*m*) with five atoms in a unit cell and a layered structure stacked

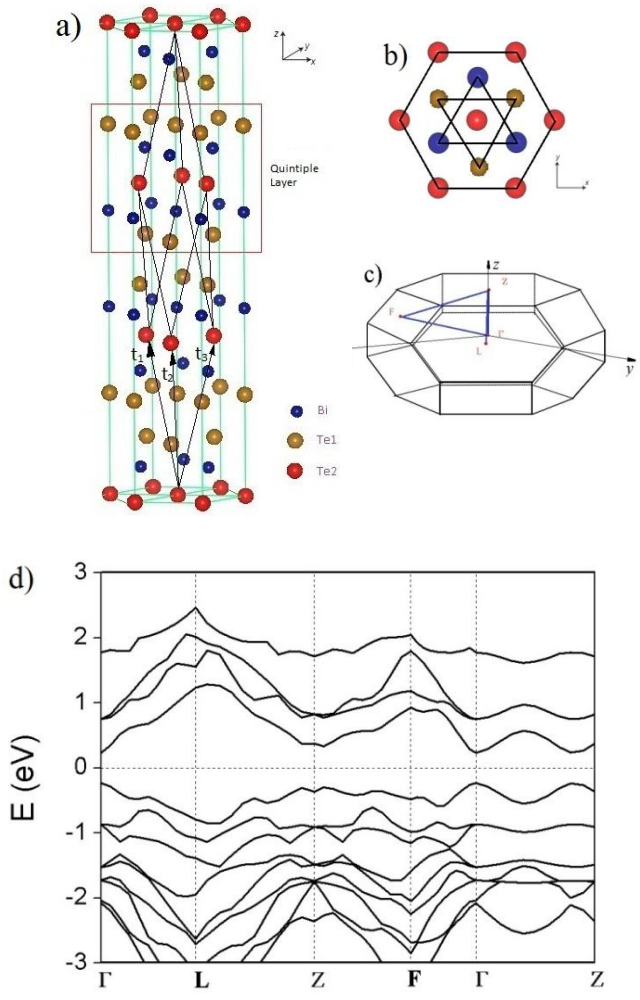


*FIG. 1. (a) Crystal structure of $Bi_2Te_3$ with three primitive lattice vectors denoted as $t_1$, $t_2$, $t_3$. A quintuple layer with Te(1)–Bi–Te(2)–Bi–Te(1) is indicated by the red square. (b) Top view along the z -direction. The triangle lattice in one quintuple layer has three different positions. (c) Bulk rhombohedral Brillouin zone and (d) electronic band structure of $Bi_2Te_3$.*

long the c-axis of the hexagonal lattice. Five-layer composed of five atoms is known as a quintuple layer (QL) and the interlayer coupling is due to the van der Waals interaction. The five individual atomic layers occur in the sequence Te(1)-Bi-Te(2)-Bi-Te(1), where the Te(1) and Te(2) are nonequivalent tellurium sites as a shown in Fig. 1(a)**.**

All of our calculations, including geometry relaxation and electronic structure calculation are performed by using density functional theory (DFT) on the basis of projector augmented wave method (PAW) [13] implemented in the VASP package [14, 15]. Perdew–Burke–Ernzerhof (PBE) approximation was employed to describe the exchange-correlation interactions [16]. An energy cutoff of 350 eV is used in the plane wave basis. A 5x5x1 and 9x9x1 *k*-sampling is generated by the Monkhorst–Pack scheme [17] for the bulk including and excluding SOC, respectively.

## III.RESULTS AND DISCUSSIONS

We calculated structural and electronic properties of $Bi_2Te_3$ including and excluding SOC. Total energy calculations showed that the optimized lattice parameters of the $Bi_2Te_3$ are $a=b$=4.44 Å and $c$=32.20 Å which are reasonably consistent with experiments ($a=b$=4.386 Å and $c$=30.478 Å). The band structure without SOC is given in Fig. 1(d) which shows a direct band gap at the Γ point of about 0.5 eV, whereas its stable surface exhibits metallic behavior from the electronic structure calculations (not shown here). The Fig. 2(a)-(d) shows atom- and spin- projected density of states (DOS) of Bi, Te(1), Te(2) and total DOS of $Bi_2Te_3$. It is found that the DOS is comparable with other theoretical result [16]. As seen in the figures, DOS near the Fermi level are determined by solely p states while s states do low energy bands. The conduction band of $Bi_2Te_3$ is mainly contributed by Bi and Te1 atoms, whereas DOS of Te2 is fully occupied. As a result, a band gap of about 0.5 eV is calculated in the total DOS in Fig. 2(d), where our result is somewhat overestimated as compared with the experiments. In order to clarify a deviation between theory and experiment, we apply the SOC term in Kohn-Sham equation by means of the DFT. The calculated DOSs with SOC are given in Fig. 2(e)-(h). DOS curves reproduced quite well with those in the previous theoretical study [18]. Main features of the valence bands are almost same, but the conduction bands are broadened to the Fermi level and higher energy region. Noting that the difference in s-DOS between with and without SOC is negligible in entire range of energy. The effect of SOC reduces significantly the band gap and very small band gap of about 0.1 eV is obtained [Fig. 2(h)]. Therefore, SOC effect should be applied to have a reliable value of band gap, i.e. narrow band gap insulator, and was found to be a decisive factor in determining of TIs.

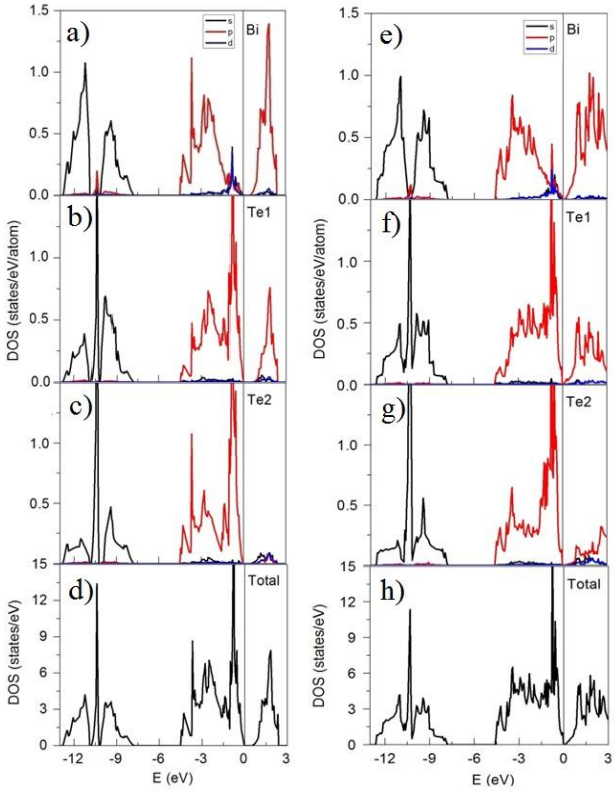


*FIG. 2. The density of states (DOS) of (a) Bi (c) Te(1) (e) Te(2) atoms in $Bi_2Te_3$ and (g) the total density of states of $Bi_2Te_3$ excluding SOC, (b) Bi (d) Te(1) (f) Te(2) and (h) total DOS of $Bi_2Te_3$ including SOC. The solid black, red and blue lines indicate s, p, d atomic spins, respectively. The vertical line at zero energy represents the Fermi level.*

## IV.CONCLUSION

The effect of SOC on the electronic structure has been considered for topological insulator $Bi_2Te_3$ alloy in framework of the first-principles DFT. The optimized lattice parameters are in good consistent with experimental and other theoretical results. The

calculated band gaps of 0.1 eV with SOC and 0.5 eV without SOC indicate that SOC gives rather consistent results with experiments. This study can be instructive to explore further investigation on new materials.

## REFERENCES

[1] J. E. Moore, Nature **464**, 194 (2010).
[2] J. E. Moore and L. Balents, Phys. Rev. B. **75**, 121306 (R) (2007).
[3] L. Fu and C. L. Kane, Phys. Rev. B. **76**, 045302 (2007).
[4] L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. **98,** 106803 (2007).
[5] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82** (2010).
[6] C. L. Kane and E. J. Mele Phys. Rev. Lett. **95,** 146802 (2005).
[7] B. A. Bernevig and S. C. Zhang, Phys. Rev. Lett. **96,** 106802 (2006).
[8] H. Zhang, C.-X. Liu, X.-L. Qi, X. Dai, Z. Fang, and S.-C. Zhang, Nature **5**, 438 (2009).
[9] S. K. Mishray, S. Satpathy, and O. Jepsen, J. Phys. Condens. Matter **9,** 461–470 (1997).
[10] S. Urazhdin, D. Bilc, S. D. Mahanti, and S. H. Tessmer, Phys. Rev. B. **69**, 085313 (2004).
[11] Y. L. Chen, et al. Science **325**, 178 (2009).
[12] Y. Xia, D. Qian, D. Hsieh, L. Wray, A. Pal, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava, and M. Z. Hasan, Nature **5**, 398 (2009).
[13] G. Kresse and D. Joubert, Phys. Rev. B **59**, 1758 (1999).
[14] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996).
[15] G. Kresse and J. Furthmüller, Comput. Mater. Sci. **6**, 15 (1996).
[16] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).
[17] H. J. Monkhorst and J. D. Pack, Phys. Rev. B **13**, 5188 (1976).
[18] P. Larson and S. D. Mahanti, Phys. Rev. B. 61, 8162–8171 (2000)