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# Effect of Hubbard Potential (*U*) on Mn Doped BiTeI

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**ABSTRACT**

In recent years, Bismuth tellurohalide has gained significant attention as a possible candidate for spintronics applications. Among them, BiTeI is one such layered material that shows Rashba spin splitting responsible for transport phenomenon. On the basis of density functional theory calculations using full-potential local-orbital code, we studied the electronic and magnetic properties of $Bi_2TeMnI_2$ compound. Our study shows an energy band gap of 1.18 eV for the parent material BiTeI. The main contribution around the Fermi level are from the Bi-6p, I-5p and Te-5p states. Upon doping Mn atom independently to Bi, Te and I site, we found that Te site is energetically most favorable. With Mn doped to Te site, the material is found to transform to ferromagnetic semiconducting state with magnetic easy-axis along [001] with magnetic moment of 3 $\mu_B$ per unit cell. The magnetic moment is found to alter interestingly with the implementation of Hubbard-potential (*U*). The value first reduces to 1 $\mu_B$ for $U = 3$ eV and starts changing with increasing value of *U*. Due to internal ferromagnetic ordering and strong correlation effect, this compound seems to be a promising candidate for spintronics and quantum computing.

**Keywords:** Band gap, Density functional theory, Density of states, Hubbard Potential, Magnetic moment.

## 1. INTRODUCTION

Bismuth tellurium iodide (BiTeI) is a fascinating ternary compound with a unique combination of elements bismuth (Bi), tellurium (Te), and iodine (I) showing intriguing electronic, optical [1-3] and topological properties [4-7] making it an important material in the field of condensed matter physics and materials science. Bismuth is a heavy metal element known for its distinctive properties, including its role in topological insulators and its relevance in the search for exotic electronic states [8]. Tellurium is a semimetal element that has properties similar to metals and nonmetals so, it is an essential component in thermoelectric materials [9] and can exhibit interesting electrical conductivity. Iodine is a halogen element that can introduce electronic and optical effects [10] into compounds, contributing to their unique characteristics. BiTeI typically has a relatively large band gap, making it suitable for applications involving optical devices and semiconductors. It is initially a large band gap semiconductor with a pronounced Rashba-type spin-orbit interaction, and it has been forecasted to transform into a robust topological insulator when subjected to moderate pressure [4] via an intermediate Weyl semimetalic phase [11, 12]. The utilization of density functional theory (DFT) with the application of *U* enhances the prediction of electronic characteristics [13] for highly correlated systems. Demonstrated by phonon dispersion analysis of transition-metal monoxides [14] it becomes evident that the DFT + *U* approach enhances electronic structures as well as vibrational features of correlated systems so we have used the DFT approach to analyze the effect of *U* on the electronic properties of Mn doped BiTeI. Effect of magnetic atom (V) doping on BiTeI is studied to find novel topological properties due to energy gap opening [15-17]. Manipulation of topological surface states and ferromagnetism on Mn doped topological insulator $Bi_2Te_3$ is studied showing the way for spintronic device application [18] so we are motivated to study the effect of magnetic doping (Mn) on BiTeI and we predict that the large band

gap semiconductor is changed to metallic ferromagnet due to the effect of *U*.

## II. METHODS

### Computational Details:

Electronic and magnetic properties are calculated in the framework of density functional theory (DFT) [19, 20] using full-potential local-orbital (FPLO) code [21]. Standard generalized gradient approximation (GGA) [22] with electron correlation effect is considered. We obtain the structure of $Bi_2TeMnI_2$ by replacing one Te atom at (−1/3, 1/3, −0.346) position with Mn atom in the (1 × 1 × 2) supercell of BiTeI having 6 inequivalent atoms in the trigonal structure with space group *P3m1* (156). Self-consistent calculations were carried out using the scalar relativistic mode. Due to the presence of Mn atom, strong effect of *U* are noted. On the basis of the reported value of *U* for Mn as 3 eV and 4 eV [23-25] so, we limited our study upto 4 eV.

### Crystal structure:

Compound BiTeI has a trigonal structure with symmetry space group *P3m1* (space group no. 156). It is a layered compound containing three inequivalent atoms of Bi, Te and I as shown in fig.1. The lattice parameter used are, $a = b = 4.425$ Å and $c = 7.378$ Å and angles $\alpha = \beta = 90^0$ & $\gamma = 120^0$. The atomic lattice positions are [0.33, -0.33, -0.08], [0, 0, -0.31] and [-0.33, 0.33, 0.21] for Bi, Te and I respectively [26].

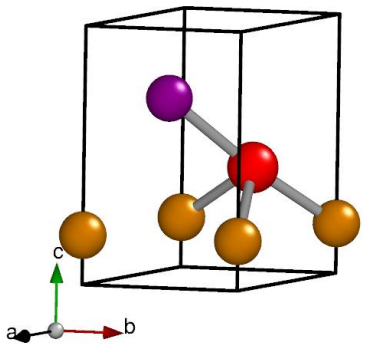


**Fig. 1:** Crystal structure of BiTeI where, Red ⇒ Bi, Yellow ⇒ Te and Purple ⇒ I

## III. RESULTS AND DISCUSSION

### Electronic properties:

We start with the study of the total and partial density of states (DOS) within GGA for the parent compound BiTeI. The partial DOS shows that Bi-6p has major contribution on the conduction band minimum and I-5p has the major contribution on the valence band maximum near Fermi level ($E_F$) whereas Te-5p has the major contribution around the $E_F$ in both the bands which can also be seen from the density of states (DOS) plot in Fig. 2 (a). The corresponding band structure is shown in Fig. 2 (b). With Mn doping to the Te site, total energy calculations are considered for non magnetic (NM), ferromagnetic (FM) and antiferromagnetic (AFM) cases.

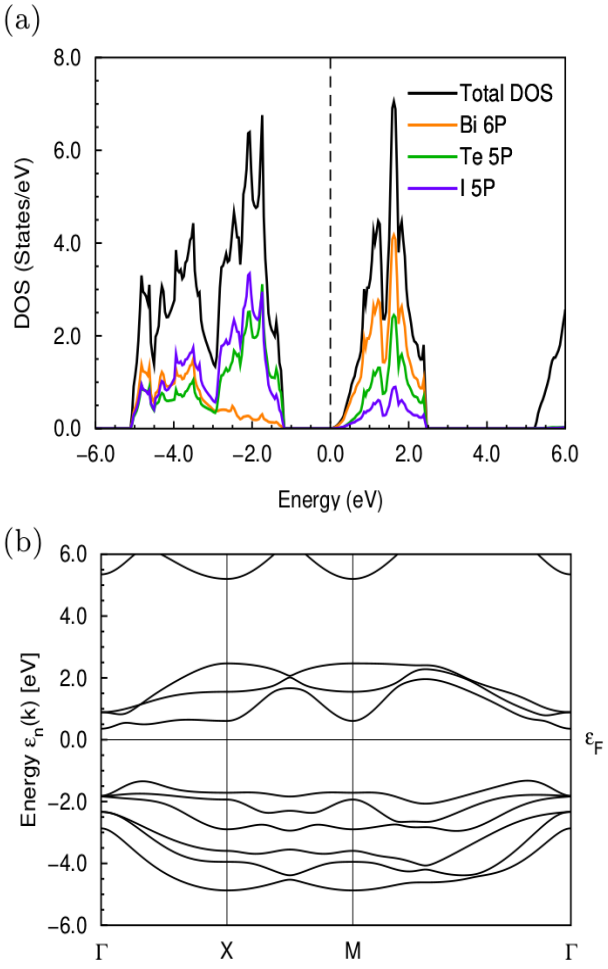


**Fig. 2:** Band and DOS plot for BiTeI in scalar-relativistic mode.

To consider the correlation effect for the Mn-doped BiTeI (i.e., $Bi_2TeMnI_2$), we performed additional calculations with GGA+*U*. We found that FM is the magnetic ground state for *U* ranging from 0 to 4 eV. The energy band gap varies significantly from $U = 0$ and reaches upto 0.3 eV for $U = 3$ eV (see Fig. 3 a-b). As soon as the *U* value rises to 4 eV, the material transforms to conducting state (see Fig. 3 (c)).

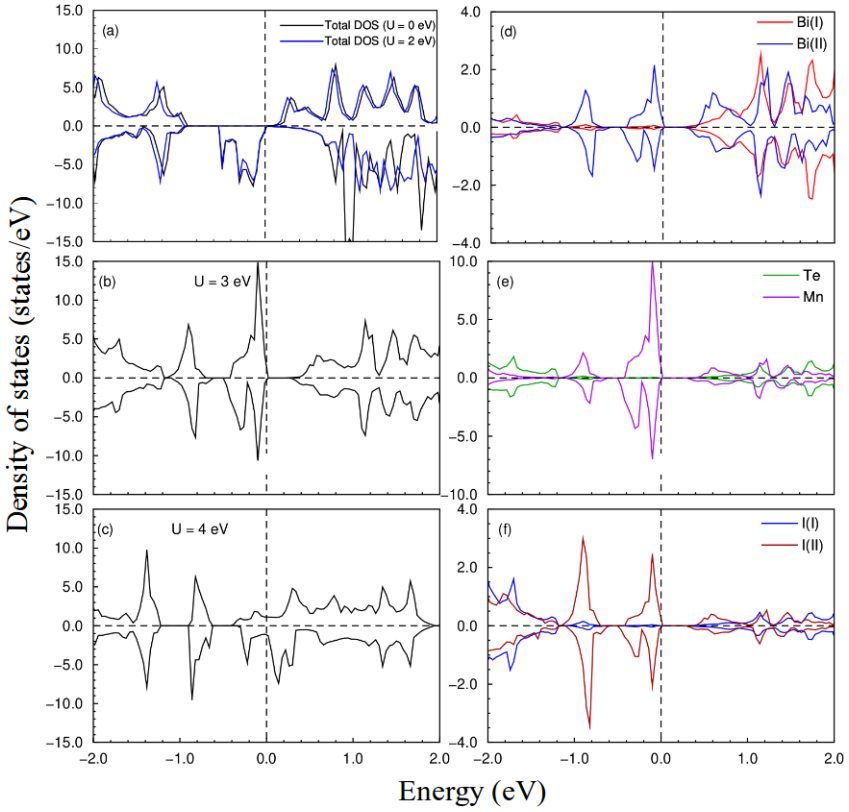


**Fig. 3:** Total and partial DOS of $Bi_2TeMnI_2$ in scalar-relativistic mode within GGA and GGA+*U* (with *U* = 2, 3 and 4 eV for Mn, respectively). Vertical dashed line represents Fermi level.

Since, the *U* value reported for Mn in literature [24] is 3 eV (for $Na_2Mn_3Se_4$) to reproduce the experimental band gap, we take this value as our benchmark to discuss the electronic and magnetic properties of $Bi_2TeMnI_2$. From the partial DOS for *U* = 3 eV as shown in Fig. 3 (d-f), the main contributions to the total DOS are found to be from the Bi (II), Mn and I (II) in the valence region close to the $E_F$ whereas Bi (I) and Bi (II) contribute mostly and Te, Mn and I (I and II) partly in the conduction region.

The partial DOS of Bi (II) and I (II) are found to hybridize strongly in the valence region around $E_F$, while Te hybridize with I (I) and Mn with I (II) in the conduction region (see Fig. d-f).

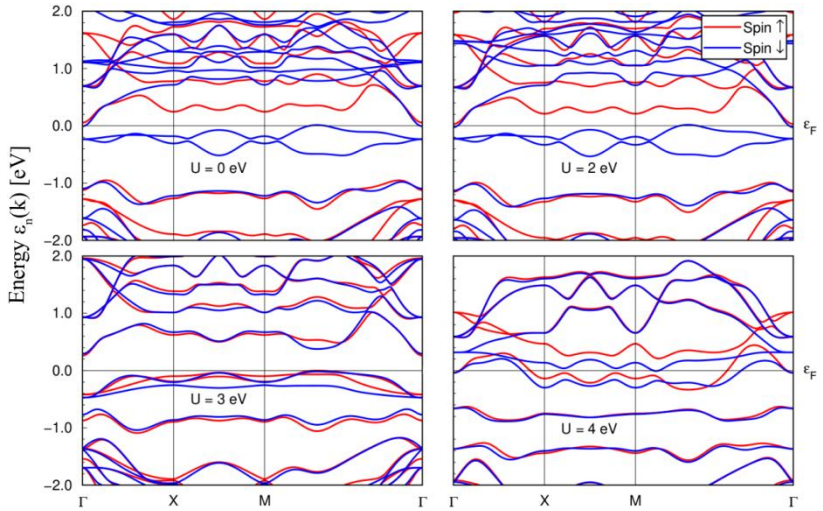


**Fig. 4:** Electronic band structure of Bi2TeMnI2 in scalar mode for different values of *U*. Horizontal solid line indicates the Fermi level.

The electronic band structure for different values of $U$ is shown in Fig. 4. As can be noted, the material is semimetallic for $U$ = 0 and 2 eV with similar nature of band, while it becomes semiconducting with an indirect energy band gap of 0.3 eV for $U$ = 3 eV, and metallic at 4 eV respectively.

**Magnetic properties:**

As discussed above, the material $Bi_2TeMnI_2$ is found to be a ferromagnet with the minimum total energy. The effective magnetic moment are mainly contributed by the Mn atoms which gives rise to magnetic polarization in Bi (II). Within GGA, the calculated effective magnetic moment is 3 $\mu_B$ per unit cell with individual magnetic moment of Mn as 4.57 $\mu_B$. The induced magnetic moment for Bi (II) is -1.21$\mu_B$. This gives rise to spin-polarization with an exchange energy of about 0.44 eV (see Fig. 3) between the spin-up and spin-down channel close to $E_F$.

The magnetic moments does not vary upto $U$ = 2 eV, however, for $U$ = 3 eV, the effective magnetic moment reduces significantly to 1 $\mu_B$ per unit cell with 1.05 $\mu_B$ per Mn atom. When $U$ increases to 4 eV, the effective magnetic moment reduces to 0.18 $\mu_B$ per unit cell.

## IV. CONCLUSIONS

In conclusion, ground state of the Mn doped BiTeI is found to be FM. Upon Mn doping, the material is transformed to metallic ferromagnet from non-magnetic semiconductor upto $U$ = 4 eV due to change in electronic band structure and altering its electrical properties. Effect of electron correlations changes the band gap at $E_F$ which can bring the electronic phase transition to the material . From this study, we predict that replacing Te by 3d elements can make a fine control on charge and spins significantly. Hence, doping influences the system by changing band gap and magnetic moment modifying its properties.

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