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Electronic and Structural, properties of ZnTe using Density Functional Theory (DFT)

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Abstract - Chalcogenides like metal Telluride have been studied for many decades for solar cell application. Recently related cubic phases like **ZnTe** are attracting wide attention for many interesting applications such as thermo-electronics and sensors. Especially **ZnTe** being a narrow direct band gap (Band gap value = 1.2eV) semiconductor is recently researched a lot owing to its wide applications on electronic, optical, magnetic and thermoelectric devices. In order to understand the fundamental properties of **ZnTe** and its closely related compounds, we have performed accurate first principle calculations based on Density Functional Theory (DFT). We have used Tight bonding Linear Muff-Tin Orbital (**TB-LMTO**) program. We have performed complete structural optimization by minimizing force as well as stress. The optimized structural parameters are found to be in good agreement with experimental values. We have analyzed electronic structure by calculating band features, site and orbital projected Density of States (**DOS**). In order to reproduce the experimental band gaps we used **LDA** (Local Density Approximation) and hybrid functional to describe its correlation effects better than usual **LDA**. The nature of bonding is analyzed using **COHP** (Crystal Orbital Hamiltonian Population) and charge density plots.

Key Words: Chalcogenids, ZnTe, DFT, TB-LMTO, LDA electronic properties, DOS, COHP.

1. INTRODUCTION

In last decade with increase in computational power, several numerical simulations are being carried out which has made it possible to predict properties (structural, electronic and optical etc.) of solids with great accuracy [1,2]. Inspite of high complexity and defective forms, II-VI group of semiconducting materials remains as the major regime of research interest in condensed matter physics because of their wide band gap nature. The cubic **ZnTe** was synthesized in solid state using 900W microwave plasma method by Tawat Suriwong et al., [4]. This semiconducting materials showed a 2.6 eV wide direct band gap has a variety of applications; green-light-emitting diodes, solar cells, waveguides, modulators [3-8], and other opto-electronic and thermoelectronic devices, Young KT et al., [5]. The compound **ZnTe** is extensively studied on its well-known structure zinc blende (**ZB**) and rocksalt (RS) and was discussed by J. Pellicer- Porres et al., [6]. In this paper, we depict various physical and electronic properties of **ZnTe** compounds by using Density Functional Theory (DFT) [7-10].

The total energy of **ZnTe** is calculated using tight binding linear muffin tin orbital method (**TB-LMTO**) [10, 11] and it has a band gap of 0.97 eV which is low when compared to experimental band gap value. So it provides a solution to minimizing the mismatch of results obtained from theoretical and experimental study. The experimental data collected from crystal open database for **ZnTe** electrical properties using DFT was discussed by Pellicer-Porres and S.K.Gupta et al., [12, 15]. From the experimental and Theoretical result it is observed that **ZnTe** exhibits **ZB** structure.

Generally zinc blende (**ZB**) structure calculation can be explained effectively with the help of available experimental data [16-18]. The elements belonging to the group of II-VI are very useful for technological applications [17, 18]. Here we have investigated the structural and electronic properties for **ZnTe** [19]. We hope that the present work will inspire the experimental group to invoke their knowledge in this particular field to analyze it experimentally [20]. The plan of the paper work is as follows section-2 gives a description about computational method followed by a result and discussion in section-3 which contains details about the structural properties, electronic band structure and **COHP** properties, finally the conclusion is given in section-4.

2. COMPUTATIONAL DETAILS

There are several methods to calculate structural, electronic and optical properties of compounds computationally. The density functional theory is one of the most accurate ways to reach acceptable results that helps us to envision the features and character of materials and nano-structure materials in particular [21]. The structural and electronic properties of (**ZnTe**) are investigated in this paper. The electronic band features of **ZnTe** in the **ZB** structure is studied using the Tight Binding Muffin Tin Orbital **(TB-LMTO)** program [22], this program calculate the Kohn-Sham eigenvalues within the framework of DFT [23]. In the calculations have been

performed with the use of local density approximation **(LDA)** [24, 25], this is includes the Coulomb interaction in the **LDA** Hamiltonian. The interaction between electrons and atomic cores is described by the non-norm conserving pseudopotentials are implemented in the **LMTO** code [26]. The pseudopotentials are generated in accordance to the linear fixed based methods [27]. The values of the parameters U and J required for the **LDA** studies were found from band structure calculations for different values of U by adjusting the position of Zn-3d bands to the experimentally compared band gap values [28].The Muffin Tin approximation makes it easier to solve the Schrödinger equation by the approximation potential [28,29]. In the **TB-LMTO** program the inputs are the crystal structure while outputs are total energy, charge- and spin-self consistent band structure, partial densities of states, Fermi surface, full charge and spin density plots, and partial pressures etc [30-33]. In this work using in this program we have calculated the total energy, band structure, total and partial densities of states and **COHP** of a **ZnTe** material.

3. RESULT AND DISCUSSSION

This study is mainly concentrated on the group II-VI metal chalcogenides and their structural, band structures and total and partial density of states and **COHP** we will calculate using density functional theory (DFT). The compounds zinc telluride (**ZnTe**) is a stable crystalline compound formed by zinc and tellurium. The **ZnTe** has face-centered cubic structure in Zinc- Blende (**ZB**) type structure with space group **F-43m (No: 216)**, (Fig.1) shows that the crystal structure of **ZnTe**. The initial guess crystal structural details are taken from experimental studies. We used lattice parameter of **a=6.07Å** with Zn and Te atoms positions is **(Zn=0, 0, 0)** and **(Te=0.25, 0.25, 0.25)**, respectively.

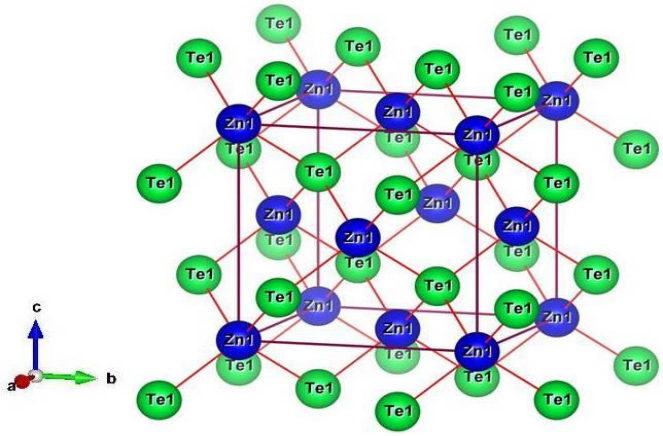

Fig -1: Crystal structure for **ZnTe**

3.1. STRUCTURAL PROPERTIES

3.1.1. K-Point Optimization

The K-point energy of the system is minimized and does not change anymore and appropriate for the calculation of physical properties of the given material. The calculated k-point energy values are **-17167.4634 eV.** We have calculated the total energy for the K-point grids starting from **2 x 2 x 2** to **12 x 12 x 12**, the Fig. 2 plot irreducible K-points and total energy and which shows that the total energy of a system does not vary significantly beyond **8 x 8 x 8** range. It is found that on further increasing the K-points, there is no change in total energy. So the K-point grid is considered to be an optimized K-point grid and it has been used to calculate the other properties of systems in our study.

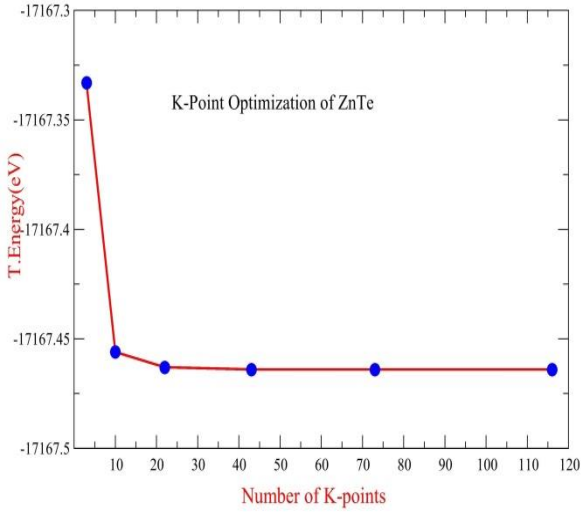

Fig -2: K-point optimization Zinc Telluride (**ZnTe**)

3.1.2. Volume Optimization

Total energy has been calculated for different volumes of crystal structure by changing the lattice parameter used in the **ZB** structure. The volume in which the system has the lowest total energy is said to be the ground state volume of the stable structure. The lattice parameter corresponding to the lowest energy structure is used to calculate further properties such as electronic and structural properties etc,. Fig.3 shows the calculated total energy with respect to different volumes of **ZnTe**. According to our calculation the **ZnTe** has the lowest total energy for the volume of 398 $Å^3$. Hence the crystal structure at this volume is used for further investigation of **ZnTe** properties.

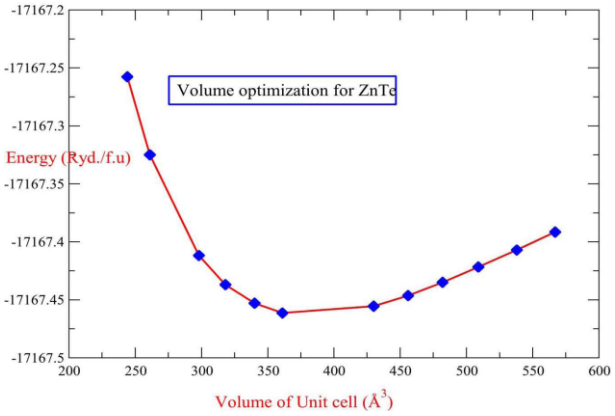

Fig -3: Volume of optimization for **ZnTe**

3.2 ELECTRONIC PROPERTIES

3.2.1 Band Structure

ZnTe is seemed to be a direct-band gap semiconductor. A closer inspection of the energy-band structure shows that the band gap is between the top of the valence band (**VB**) at the Gamma (G)-point and the bottoms of the conduction band (**CB**) at the Brillouin zone (BZ) point. As the unit cell contains 46 atoms the band structure is quite interesting it is shown in Fig.4. In this band structure the energy range is from -15 to 15 eV. There is a finite energy gap at 0.97 eV between the topmost-occupied **VB** and the bottommost -unoccupied **CB**. We are interested in increasing the band gap value which would be near to the experimental band gap value, so we are applied Local density Approximation (LDA). Now its band gap value (1.2 eV) increased which is near to experimental band gap value 2.26 eV [2].

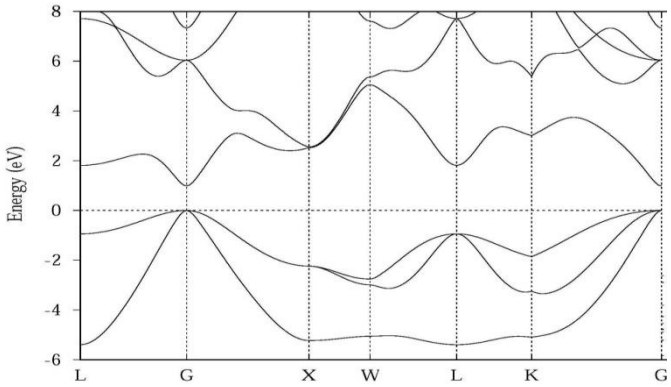

Fig -4: The electronic band structure of **ZnTe**. The line at 0 eV refers to Fermi energy level

For the purpose of more clarity, and convenience the most occupied portion of the band structure (Fig.4) in the valence band (**VB**) is divided into two regions: (i). Bands lying at below -6 eV. (ii). bands lying top of the **VB**, and closer to Fermi Level (E_F), viz., -5 to 0 eV. Region (i) contains the bands with contributions from **Te-s, d** and **Zn-s, d** electron from Fig.5 for **DOS**. Second region includes more bands lying on the most occupied **VB**. These bands are due contributions from **Te-p, d** and **Zn-s, p** and **d** contain more electrons from (Fig.5) **DOS**. In the unoccupied portion of the band structure a corresponding division leads to two energy regions: (i) The bottommost **CB** from 0 to 12 eV and (ii) Above 12 eV the one band will be appearing. There are 4 bands in region (i) with have some **Zn-s, p**; **Te-s, p** and **d** electrons form Fig.5. The region (ii) the bands **Zn-p** band only most occupied in the **CB** above 12 eV.

3.2.2 Density of States (DOS)

The important description of the electronic structure for many purposes is provided by the density of states (**DOS**) which is another way to visualize and analyze the electronic structure. The **DOS** D(E) is the number of states in the unit energy range

$$D(E) = \frac{dN}{dE} = \left(\frac{V}{2\pi^2}\right)\left(\frac{2m}{\pi^2}\right)^{3/2} E^{1/2}$$

The maximum D(E) at **T=0** corresponds to the Fermi energy at the ground state, when T ≠ 0, the electrons occupy higher energy states. The Fig.5 shows the total **DOS** for **ZnTe**. Total **DOS** also reveals the band gap obtained in the band structure and the valence band spread which over -13 eV to 0 eV in the energy ranges. The top of the valence band has highly localized states around over the -8 eV. In the localized peak of **DOS** is seen in the Partial **DOS** in shown in the Fig.6 where the conduction Fig. 5 total density of states (**DOS**) for **ZnTe** in the Fermi line set to zero and **ZnTe** configurations of **s, p, d** states band is spread from Fermi line set as zero. The above Fermi line called conduction band and below is defined as valence band, so our convenience we shown the **DOS** from 0 to 15 eV range in the conduction band.

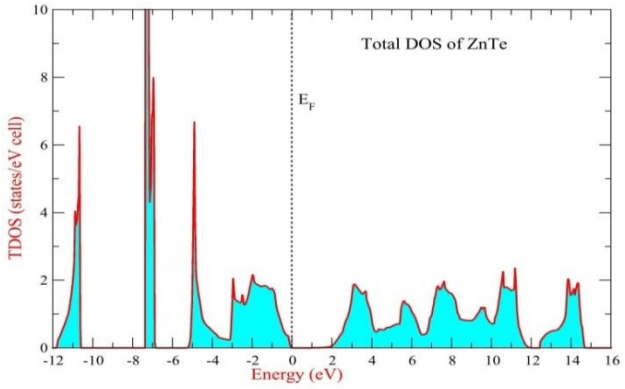

Fig -5: Total Density of States (**DOS**) for **ZnTe** in the Fermi line set to zero and **ZnTe** configurations of **s, p, d** states

From the partial **DOS** analysis, we found that the peak is due to the localization of **d** electrons of **Zn** and **Te** and **p** elections of **Te.** The origin of the top of the **VB** was mostly due to the **s** electron of **Zn** and **p** electron of **Te** which led to a further conclusion for the possibility of **s-p** hybridization. The results show from Fig.7 covalent bonding nature as the ZnTe.

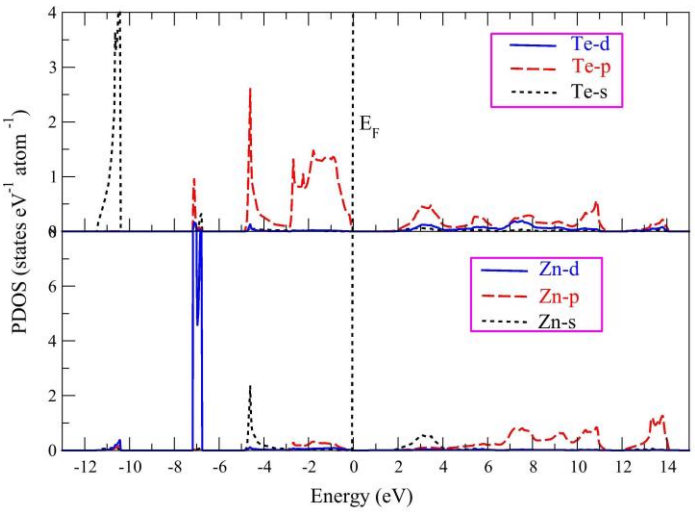

Fig -6: Partial Density of States (P**DOS**) **ZnTe** in the ground-states configurations. The Fermi level is set to zero.

The Fig.6 it shows the partial **DOS** of **ZnTe** the top of the valence band is complete band whereas conduction bands is partially filled and empty bands.

The top of the valence band contains **s** band of tellurium with 40 states/eV its means that contributions of electron for the conduction between the **CB** and **VB** is from the **s** band of tellurium. The **d** band for zinc and **Te** it's delocalized in the bottom of the valence band, it type of bands don't help to conduction of electrons, because its bottom of the valence bands.

3.2.3. Crystal Orbital Hamiltonian Population (COHP)

Another useful tool to distinguish bonding, anti-bonding, and non-bonding interaction between atoms is the crystal orbital population (**COHP**). According to this **COHP** concept negative **COHP** values indicate bonding, positive values antibonding, and zero **COHP** together with finite **DOS** value suggests non-bonding states. The **COHP** is a quite meaningful way to measure the effective strength of bond interactions. The calculated **COHP** for Zn and Te are displayed in Fig. 7. For both Zn and Te atoms the **VB** consists of bonding states and the **CB** of anti-bonding states indicating that both have strong bonding interaction with the both atoms. The integrated **COHP** value (it's provides a measure of bond strength) for 1.53 eV. Here the cubic **ZnTe** atoms have stronger bonding interaction with Te

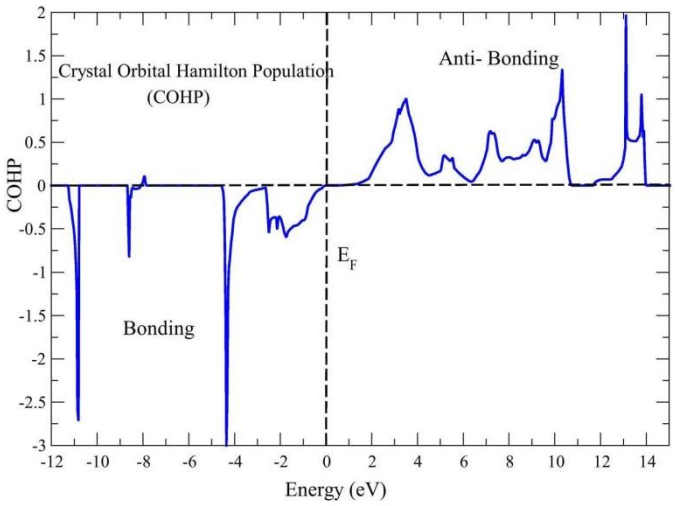

Fig -7: Calculated **COHP** curves for **ZnTe**

4. CONCLUSIONS

The first principle Tight Binding- Linear Muffin Tin Orbital **(TB-LMTO)** and linear fixed based method was used to investigate the structural properties and stability of the **ZB**. The experimentally measured lattice parameter and band structure parameters for **ZnTe** have been are used **TB-LMTO** calculations with the **LDA** approximation. It is shown **ZnTe** is direct band gap semiconductor material and its band gap value is 0.97 eV. The band gap was increased using **LDA** its band gap value is 1.12 eV. The **DOS** and P**DOS** graph showed that the result was with good agreement with experimental values. The band dispersion between the **VB** and **CB** was also discussed with the experimental values. The **COHP** figure showed the bonding states between the **CB** and **VB** along with the integrated CHOP values.

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