# DFT investigation of electronic, optical, mechanical and thermoelectric properties of ZnTe

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**Abstract:** Using full-potential linearized augmented plane wave (FP-LAPW) method, the structural, electronic, mechanical, optical and thermoelectric properties of ZnTe are studied in Zinc-blend structure at ambient conditions. All the calculations are carried out by using Density Functional Theory (DFT) implemented in Wien2k code, where the exchange-correlation functional is approximated using the Generalized Gradient Approximation (GGA). The DFT calculation produces better results for ground state properties lattice constant, volume, bulk modulus and total energy of ZnTe agreed well with available theoretical and experimental values. The ZnTe possess a direct band gap at the 'Γ' symmetry point with calculated energy gap value 1.03 eV revealing their semiconducting nature. The mechanical properties namely, Young's modulus, Shear modulus, Poisson's ratio and Hardness are also calculated. Based on the ductile/brittle analysis, ZnTe identified as ductile material suitable for flexible wearable thermoelectric applications. Using semiclassical Boltzmann transport theory, the thermo-efficiency of the material is analyzed based on the calculated thermoelectric properties namely Seebeck coefficient, electrical conductivity, power factor and figure of merit. The optical properties absorption, optical conductivity, eloss, dielectric constants, reflectivity and refractive index were calculated for the energy range between 0 - 13.98 eV.

**Keywords**: DFT, Wien2k, II-VI Semiconductor, Band Structure, Elastic constants

## Introduction

In the last few decades, the vast industrial applications of zinc-chalcogenide semiconductors (ZnS, ZnSe and ZnTe) have attracted much attention due to their wide and direct band gap, unique structural and electronic properties. Among these materials, ZnTe has a somewhat narrower bandgap [1] and is stand up for applications such as thin-film solar cells [2], radiation detectors, and heterojunction-based devices, where its excellent p-type conductivity plays a key role. ZnTe crystallize in the zinc blende structure [3-6] and exhibit strong covalent–ionic bonding, contributing to their excellent stability with good ductile nature[3]. The ductile semiconductors are salient materials in flexible thermoelectric applications, since the fabrication of flexible thermoelectric devices using ductile thermoelectric semiconductors is big challenging due to the lack of good p-type ductile thermoelectric materials. Hence, in this present study, the ductile/brittle analysis and thermo-efficiency of ZnTe focused mainly.

DFT-based studies have been significant in investigating the electronic band structures, charge distribution, mechanical properties, and optical response functions of the materials, aiding in the design and optimization of optoelectronic devices, solar cells, thermoelectric and other applications [5]. Several studies have explored both theoretical and experimental aspects of Zn-chalcogenides, providing valuable insights into their potential for various applications. Early investigations primarily focused on the electronic band structures and density of states (DOS) of the materials, revealing key details about their semiconductor behaviour and optical transitions.

Bahloul et al., [7] studied the structural, electronic and optical properties of ZnTe. Erum et al., [8] explores the structural, electronic, optical, and thermoelectric properties of ZnS and ZnTe using the FP-LAPW method with DFT, revealing direct band gaps of 3.5 eV (ZnS) and 2.3 eV (ZnTe), with major contributions from the p states of S/Te and d states of Zn in the DOS. Laim et al., [9] investigated wurtzite ZnX (X = S, Se, Te) alloys were studied using FP-LAPW and mBJ potential. Mohammad Bilal et al., [10] discussed the structural, elastic, electronic and optical properties of Zn-chalcogenides under pressure. Perin et al., [11] ZnX and CdX (X = S, Se, Te) bilayers show visible band gaps, tunable electronic properties, and exciton binding energies, with ZnTe/CdS transitioning from type-I to type-II under strain. Gul et al. [12] finds that the tetragonal phase of ZnTe offers the highest thermoelectric performance (ZT = 0.387 at 500 K), while the zinc-blende phase excels in optical properties for optoelectronic applications. Isik et al., [13] synthesised ZnTe thin films using magnetron sputtered method and discussed temperature tuned band gap. Singh et al., [14] studied the structural and optical properties of ZnTe thin films. Tan Jia-Jin et al., [15] investigated the pressure induced phase transition and phonon spectrucm of zinc blend II-VI semiconductors ZnX(X=S, Se, Te).

Here, zinc blend chalcogenides are chosen as the parent base materials for the present study. The aim of the study is to enhance the ductility with good thermoefficieny of the zinc-based chalcogenides ZnX (X=S,Se,Te) by doping and co-doping method for flexible thermoelectric applications. First, the study has been initiated for the insights of parent binary zinc chalcogenides ZnX (X = S, Se, Te). The analysis of ZnSe has been completed in our previous paper. In this study, we have reported the complete analysis of ZnTe includes structural, electronic properties- band structure and density of states, elastic properties, mechanical stability with ductile/brittle analysis, optical properties for opto-electronic applications and thermo-efficiency for thermoelectric applications.

**Methodology**

First principles calculations are carried out using Density Functional Theory [16] implemented with Wien2k [17] code to study structural, electronic, mechanical, optical and thermoelectric properties of ZnTe.

The structure of ZnTe has been optimized by PBE-GGA [18,19] (Perdew-Berke Ernzerhof - Generalized Gradient Approximation) exchange potential. The muffin-tin sphere radius for zinc is 2.42 and for tellurium is 2.15. The Zn - $4s^2\ 3d^{10}$ and Te - $5s^2 4d^{10}\ 5p^4$ are considered as valance electrons. The basis sets $R_{MT} \times K_{max} = 7.0$, $l_{max} = 10$ and the $G_{max} = 12$ have been selected for accurate calculations. For total energy convergence, 1000 k-points have been considered to control a mesh of 10 x 10 x 10. The structure of the material has been visualized by XCrySDen graphic code. Using BoltzTraP [20] code the thermoelectric properties are calculated.

**Results and Discussions**

**Structural Properties**

The zinc blend ZnTe possesses cubic structure (space group F-43m) belonging to the space group number 216 shows in Figure 1a and the structural information are given Table 1. The optimized lattice constant is obtained through total energy minimization and the calculated total energy for different lattice constants are used in Birch-Murnaghan equation of state to attained the ground state properties lattice constants, volume, bulk modulus and pressure derivative bulk modulus shown in Table 2 and the volume optimization curve is shown in Figure 1b. The calculated lattice constant $a_0$ = 6.1968 ($A^0$) and bulk modulus = 43.172 (GPa) are good agreement with reported values. The binary ZnTe is a semiconducting material with direct band gap of 1.03 eV (PBE-GGA) located at 'Γ' symmetry point where valence band maximum (VBM) and conduction band minimum (CBM) are meet at same point.

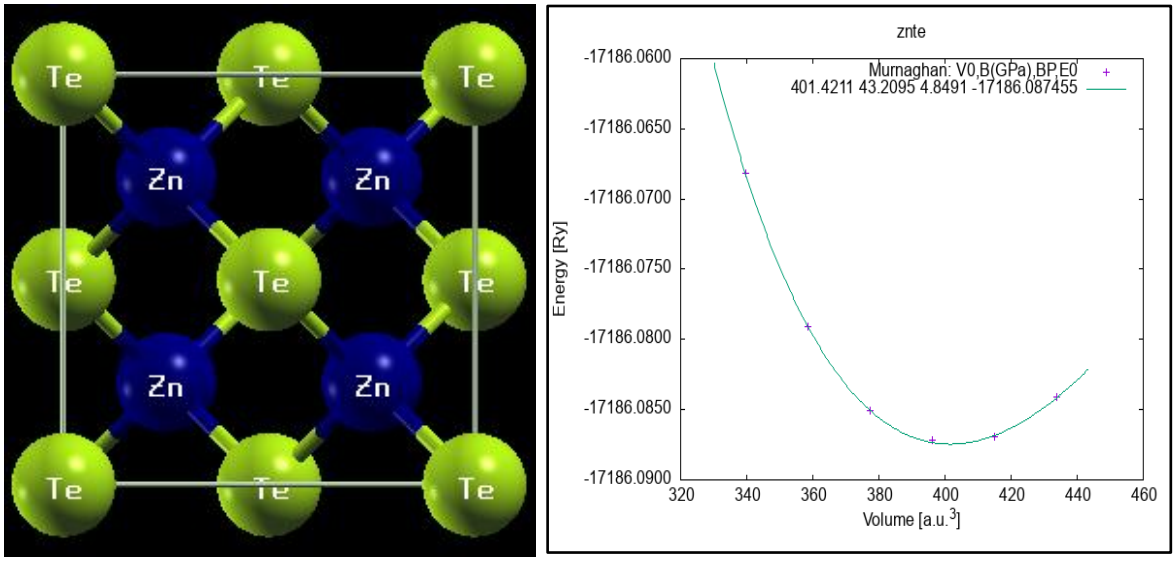



*Figure 1. (a) Structure and (b) volume optimization curve of ZnTe*

*Table 1. Structural properties of ZnTe*

| Parameter/ Alloy | Atomic Position | Structure | Space group | No. of atoms in unit cell | $E_g$ (eV) | NOE | $E_F$(Ry) |
|---|---|---|---|---|---|---|---|
| ZnTe | Zn (0.25,0.25,0.25) Te (0,0,0) | Cubic | 216 - F-43m | 2 | 1.03(GGA) | 28 | 0.24451(GGA) |

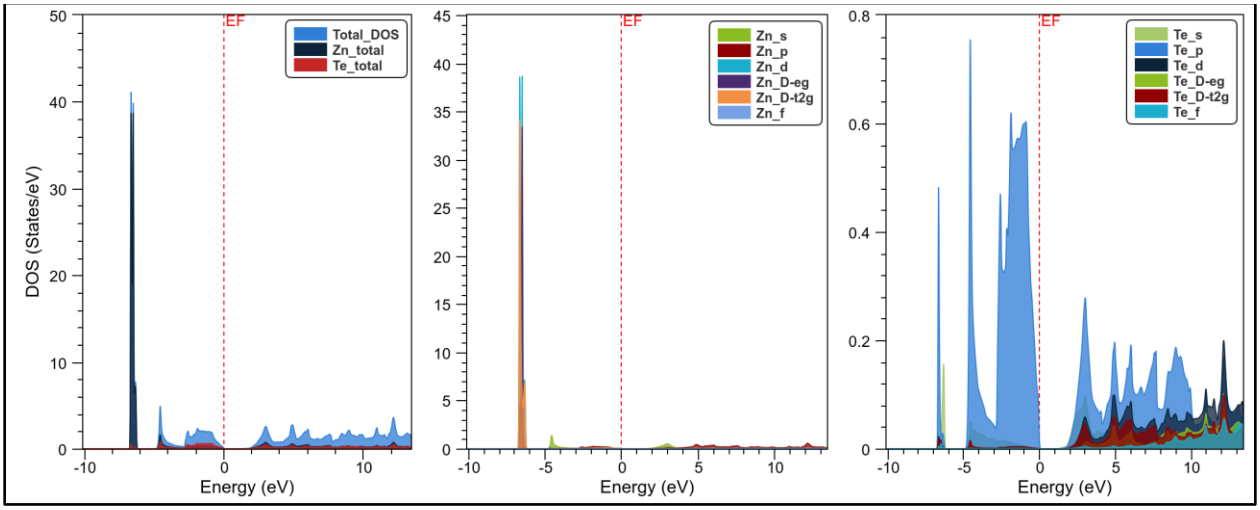
*Table 2. Calculated lattice parameter $a_0$ ($A^0$), Volume (a.u.)$^3$, bulk modulus B(GPa), pressure derivative bulk modulus B' and total energy $E_0$ (Ry) for ZnTe*

| Parameter/ Alloy | $a_0$ ($A^0$) | V (a.u.)$^3$ | B(GPa) | B' | $E_0$ (Ry) |
|---|---|---|---|---|---|
| ZnTe | 6.1968<br>6.103(exp)<br>6.078[10]<br>6.19 [26] | 401.464 | 43.172<br>51.23[10]<br>41.1[26] | 4.742<br>5.33[26] | -17186.087455 |

**Electronic Properties**

**Density of States**

The density of states histogram for ZnTe (PBE-GGA) shown in Figure 2 . In Figure 2, it is clearly shown that below the fermi level is mainly due to Zn - s, d states and Te- p states; above the fermi level is mainly due to Zn - s states; less contribution from p states and Te-s, p states. Around the fermi is mainly due to Zn -s and Te-p states. The sharp peak below the fermi level is observed at -4.8 eV. The physical properties of the materials are changed by sharp peak, here it is governed by Zn - d states.




*(a)*

*Figure 2. Total and partial density of states of ZnTe (PBE-GGA)*

**Band Structure**

The calculated energy band structure for ZnTe (PBE-GGA) shown in Figure 3. The detailed analysis has been done by fat band structure of Zn and Te all states shown in Figure 4 and 5 respectively.

The bottom region below the fermi energy level -

(i) around -6 eV in valence band is purely by Zn- d, d-eg, d-t2g states shown in Figure 4d, 4e, 4f

(ii) around -2.4 eV is mainly due to Zn - p and Te -p states; there is less contribution from Zn-d, d-t2g states

(iii) around -12 eV is mainly due to Te - s, p states

The top region above the fermi energy level -

(i) around 5.5 eV is mainly due to Zn -s, p states and Te- s, p states

(iv) around 7.0 eV is mainly by Zn-p states

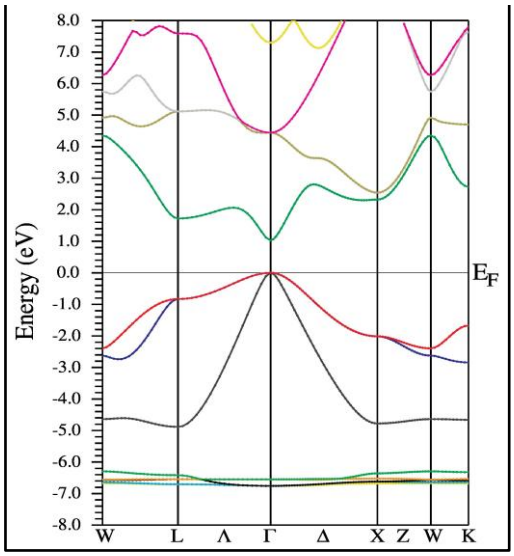



*Figure 3. Energy band structure of ZnTe (PBE-GGA).*

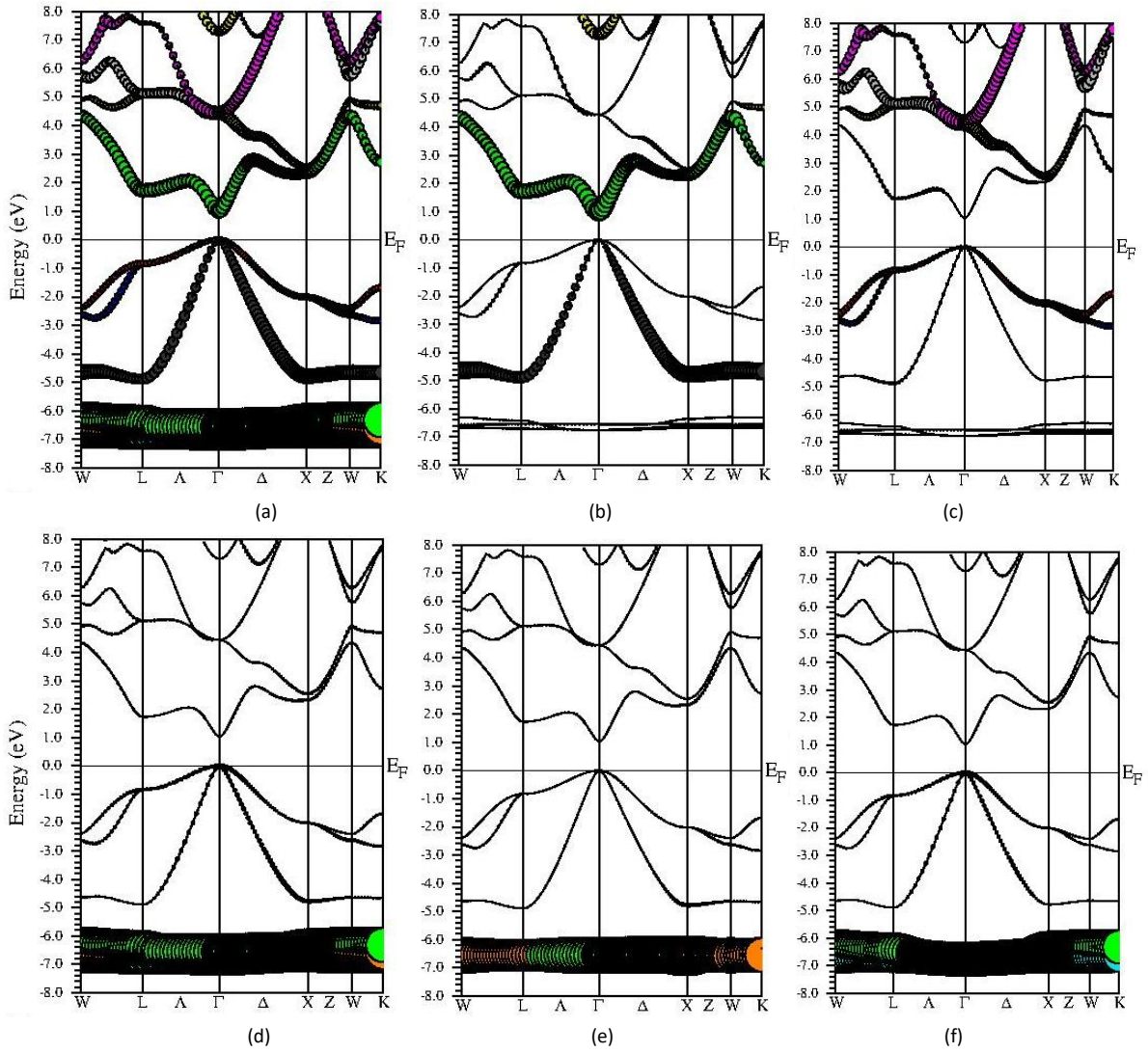



*Figure 4. fat band structure of Zn a) total b) s- c) p- d) d- e) d-eg f) d-t2g states*

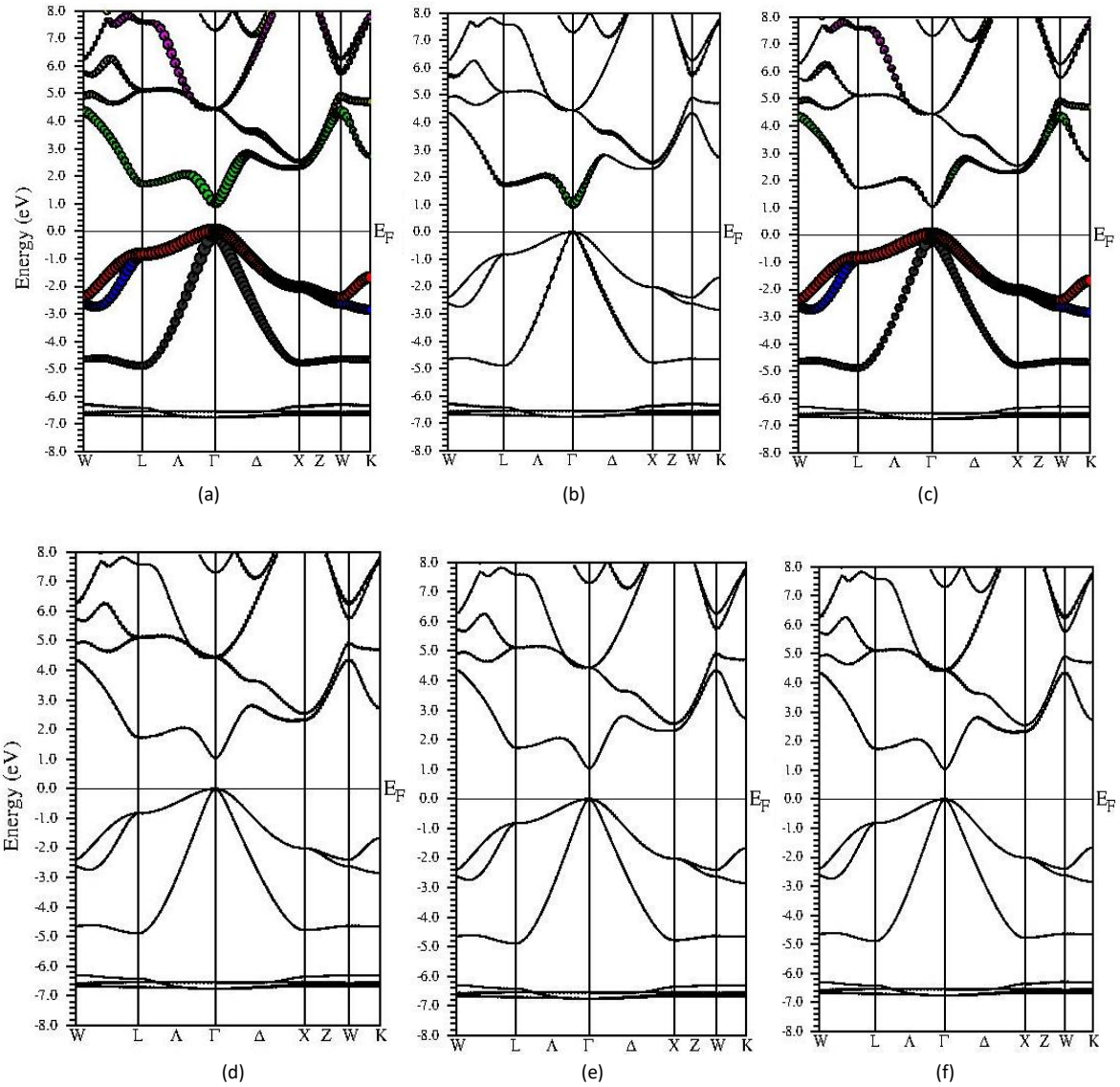



*Figure 5. fat band structure of Te a) total b) s- c) p- d) d- e) d-eg f) d-t2g states*

**Elastic, Mechanical and Thermal Properties**

The mechanical responses of the materials are analysed by using the elastic constants. For a cubic system, three independent elastic constants namely $C_{11}$, $C_{12}$ and $C_{44}$ are required to calculate the mechanical properties [21]. The elastic constants $C_{11}$, $C_{12}$ and $C_{44}$ are calculated by using IR-elast package [22] for ZnTe are given in Table 3. The properties of the materials can be defined using these constants and give the information about brittleness, ductility, hardness, stiffness, and mechanical stability of the materials. The mechanical stability of cubic material should satisfy Born's stability criteria such as $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$. Furthermore, the calculated elastic moduli also satisfy the cubic stability condition $C_{11} > B > C_{12}$. Mechanical properties such as Cauchy's pressure ($C_{12}$-$C_{44}$), Young's modulus (E), Shear modulus (G), Bulk modulus (B), G/B ratio, Vicker's micro hardness ($H_v$) and Poisson's ratio (v) are calculated and tabulated in Table 4.

From the calculated results, we have identified ZnTe is a ductile material which is confirmed by the G/B ratio of 0.51 and Poisson's ratio 0.32 with hardness becomes medium. Kleinman parameter describes the relative tendency of bond bending to bond stretching. Usually, its value lies between 0 to 1; 0 - showing minimum bond bending and 1 - showing minimum bond stretching. The value of Kleinman parameter is 1.08 for ZnTe indicates that bond bending is preferred in this material.

Elastic constants are used to measure thermal properties of ZnTe material. Debye temperature ($\theta_D$) has been calculated from average sound velocity $\boldsymbol{\nu}_m$ which is used to investigate the behaviour of the heat capacity of solids. In our previous study, the detailed formulas are discussed for ZnSe.

Also using these elastic constants, another important thermodynamic parameter melting temperature for these materials can be calculated by using the below equation

$$T_m\,(K) = 553\ K + (5.911\ \text{K GPa}^{-1})\ C_{11} \pm 300\ \text{K} \qquad [1]$$

From Table 5, we have noted lower Debye temperature, large Grüneisen parameter and maximum melting temperature, it indicates weak covalent nature of ZnTe material.

*Table 3. Elastic Constants of ZnTe*

| | $C_{11}$ (GPa) | $C_{12}$ (GPa) | $C_{44}$ (GPa) |
|---|---|---|---|
| ZnTe | 57.39<br>62.95[10]<br>64.7[15] | 37.19<br>40.62[10]<br>36.0[15] | 37.47<br>43.16[10]<br>40.1[15] |

*Table 4. Mechanical properties of ZnTe*

| | $C_{12}$-$C_{44}$ (GPa) | B (GPa) | G (GPa) | E (GPa) | G/B | ν | $H_v$ (GPa) |
|---|---|---|---|---|---|---|---|
| ZnTe | -0.28 | 43.92<br>57.3 [26] | 26.52<br>24.3 [26] | 66.24<br>64.42[10]<br>63.8[26] | 0.51 | 0.32<br>0.28[10]<br>0.31[26] | 3.819 |

*Table 5. Thermal properties of ZnTe*

| Parameter/ Alloy | $V_L$ (m/s) | $V_S$ (m/s) | $V_m$(m/s) | $\theta_D$ (K) | Tm(K) | ξ |
|---|---|---|---|---|---|---|
| ZnTe | 3696 | 2032 | 2265 | 217 | 1192 | 1.6 |

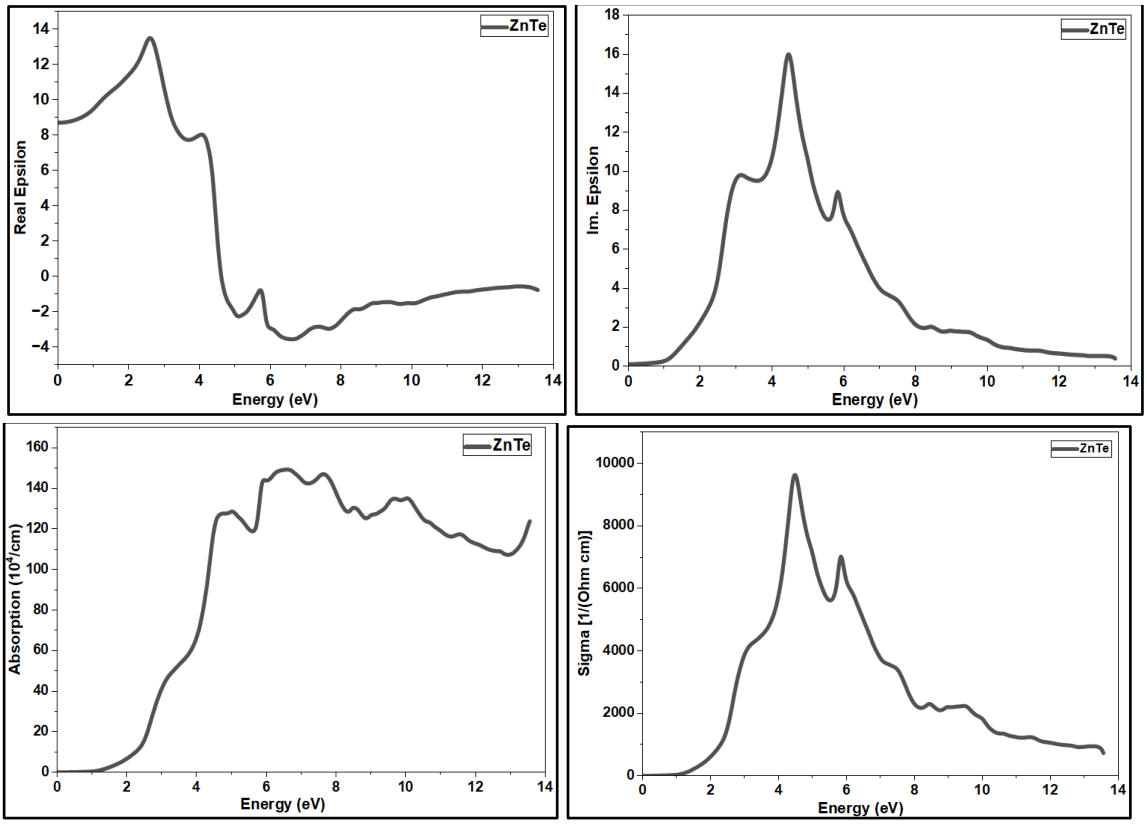
**Optical properties**

An optical property of semiconductor is an important property because of its applications in optoelectronics, solar cell, infrared detectors and switching devices, etc., All the optical properties [23] such as complex dielectric functions (real and imaginary), absorption coefficient, conductivity, reflectivity,

refractive index and optical energy loss function are calculated using the GGA approximation and the results are analyzed and presented in Figure 6 (a-g).

From Figure 6, we have noted that the real and the imaginary part of dielectric function of this material in between wide energy range from 0 eV to 13.98 eV as shown in Figure 6a & 6b. The real part attains maximum (13) at 2.5 eV and becomes negative (-2) at 5.5 eV. Optical conductivity can be calculated from the imaginary part of dielectric function and attains maximum optical conductivity value in the visible region at 4.5 eV. The maximum value of reflectivity reached the energy 8.0 eV. Energy loss becomes maximum at high photon energy.

Also we have noted that good optical absorption of the ZnTe with a wide energy range 0 -13.98 eV and are potential material for optoelectronic devices in ultraviolet (UV) region. The maximum absorption coefficient was observed at 7.5 eV. The refractive index value lies between 0.15 to 2.8 with an energy range of 0 eV to 13.98eV.



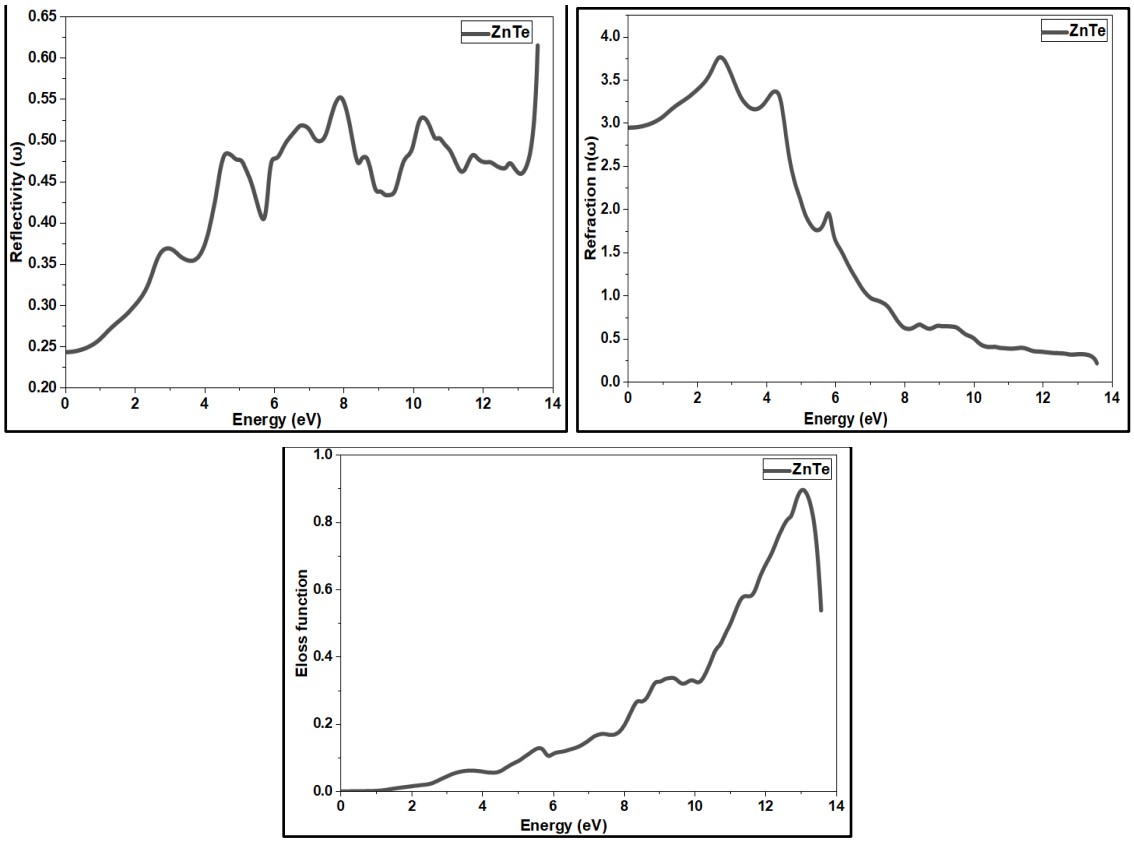



*Figure 6. Optical properties of ZnTe*

**Thermoelectric properties**

Thermoelectric properties of ZnTe material are studied at room temperature by using semi-classical Boltzmann equation implemented in Boltztrap interfaced with Wien2k and the results are tabulated.

Good efficient thermoelectric material [24] has maximum Seebeck coefficient, maximum electrical conductivity and low thermal conductivity, then the figure of merit increases spontaneously according to the formula,

$$ZT = \frac{S^2 \frac{\sigma}{\tau} T}{k_e + k_l} \quad [2]$$

Where S is the Seebeck coefficient, σ is the electrical conductivity, τ is the relaxation time, T is the temperature, $k_e$ is the electronic thermal conductivity and $k_l$ is the lattice thermal conductivity. Metal chalcogenide-based materials are very high attention, especially concerning thermoelectric properties due to their appropriate electronic and atomic structures.

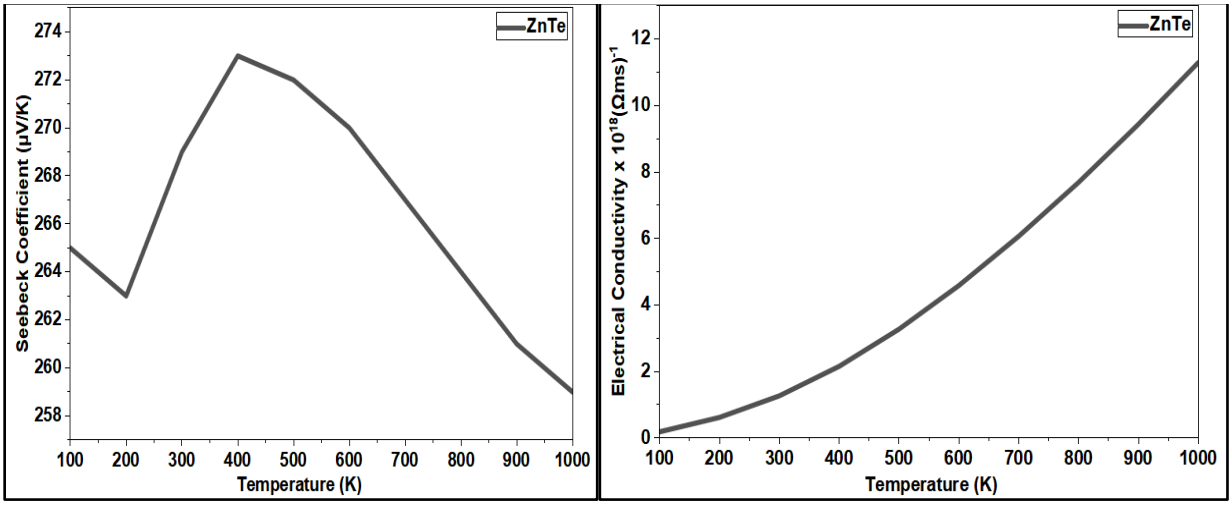
From the Table 6, the positive Seebeck value indicates that ZnTe is a p-type semi conducting material. From the results, ZnTe has reached the maximum power factor due to the thermal excitation of positive electrons (holes) and is very suitable for thermoelectric applications. Also, we noted electronic specific heat, Hall Coefficient and Pauli magnetic susceptibility at 300 K.

*Table 6. Thermoelectric properties of ZnTe at 300 K for Fermi energy*

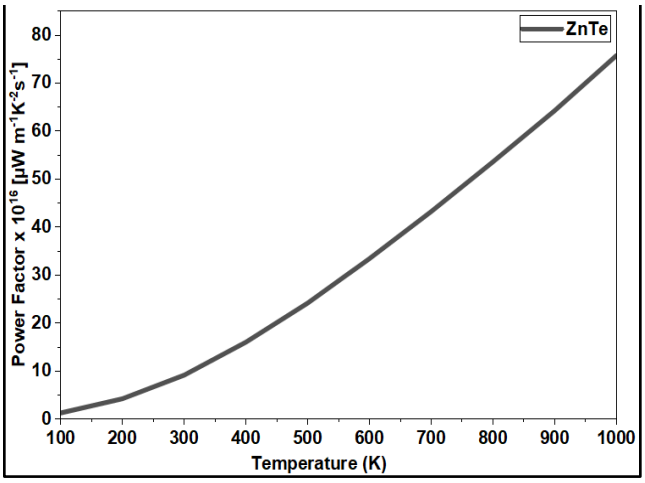
| Parameters | ZnTe |
|---|---|
| Seebeck Coefficient (S) (μV/K) | 269 |
| $\sigma/\tau \times 10^{18}$ [1/(Ω m s)] | 1.269 |
| $S^2 \sigma/\tau \times 10^{16}$ [μW $m^{-1}$ $K^{-2}$ $s^{-1}$] | 9.182 |
| Thermal Conductivity ($\kappa^0$) x $10^{12}$ [W/(m K s)] | 36.138 |
| Electronic Specific Heat ( c) [J/(mol K)] | 0.0741 |
| Hall Coefficient ($R_H$) x $10^{-7}$ [$m^3$/C] | 2.1608 |
| Pauli Magnetic (χ) x $10^{-11}$ [$m^3$/mol] | 2.2826 |

Figure 7 shows the temperature vs seebeck coefficient, electrical conductivity, power factor. In Figure 7a, the seebeck coefficient first decreases and increases then decreases upto 1000K.From 100K to 200K, seebeck coefficient value decreases, then starts to increases from 200K to 400K; finally it decreases from 400K to 1000K. Electrical conductivity is a measure of a material's capability to move electric charge carriers throughout the material. In general, electrical conductivity is a measure of Electrical conductivity increases continuously from 100K to 1000K.

Figure of merit (zT) determines the thermo efficiency of the material and it depends on the S, σ, $\kappa_e$ and T. For a good thermoelectric material, the material should have a high S and σ and low $\kappa_e$ values.




(a) (b)




(c)

Figure. 7 Seebeck coefficient, Electrical conductivity, Power Factor of ZnTe

**Conclusions**

In this work, the density function theory is employed to calculate structural, electronic, elastic, mechanical, optical and thermoelectric properties of zinc Telluride using Wien2k code. From the detailed band structure analysis and density of states histogram, we have identified the semiconducting nature of ZnTe with direct band gap value $E_g$ = 1.03 eV for GGA. The above results have been assessed by DOS histograms and the major influences around the fermi level are from Zn- s and Se -p states. The elastic parameters calculations confirmed the stability of the material. Based on the ductile/brittle analysis, the zinc blend chalcogenide ZnTe identified as ductile material with less hardness. The optical responses of ZnTe calculated for the incident photon energy up to 13.98 eV to analyses their optical behavior. The optical conductivity (sigma) and eloss are two important considerations in optical property explanation. Here, the maximum energy loss occurred at higher photon energy and maximum sigma occurred at lower photon energy reveals ZnTe is suitable for opto-electronic devices in visible and ultraviolet (UV) region. Thermoelectric properties have been calculated using BoltzTraP code implemented with Wien2k software. The calculated positive seebeck coefficient S = 269 (μV/K) indicates the ZnTe is a p-type semiconducting material. The calculated power factor for ZnTe is 9.182 ($\mu W\ m^{-1}\ K^{-2}\ s^{-1}$). From the study, it is concluded that the studied ZnTe material is a ductile p-type thermoelectric material which is a suitable material for flexible wearable thermoelectric applications.

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