Computational insight into the structural, electronic, mechanical, optical and thermoelectric properties of ZnSe - DFT Study

Manjula Muthurathinam[1], Chandra Kumar Dixit[2], Shasi Kant Gupta[3] and Muthumari Muruganantham[4]

[1] Post Doctoral Researcher, Lincoln University College, Malaysia

[2] Director, Institute of Engineering & Technology, Dr Shakuntala Misra National Rehabilitation University, Lucknow, India 226017

[3] Adjunct Professor, Lincoln University College, Malaysia

[4] Assistant Professor, Jerusalem College of Engineering, Chennai-600100, India

Email ID: pdf.manjula@lincoln.edu.my

Abstract: Flexible thermoelectric materials are receiving more attention than bulk thermoelectric materials due to their capacity of converting heat into electricity directly along with easily contact with curved heat sources. The present study mainly focused on the structural, elastic, mechanical, optical and thermoelectric properties of Zinc-based binary chalcogenide ZnSe belongs to II-VI semiconductors by means of Density Functional Theory (DFT) using Wien2k software. The DFT calculation produces better results for electronic and transport properties of II - VI semiconductors. The obtained ground state properties lattice constant, volume, bulk modulus and total energy of ZnSe agreed well with existing theoretical and experimental values. The zinc blend cubic ZnSe possess a direct band gap at the Γ with calculated energy gap value 1.061 eV revealing their semiconducting nature. The thermoelectric properties namely Seebeck coefficient, electrical conductivity, lattice thermal conductivity, power factor and figure of merit have been calculated for ZnSe using semiclassical Boltzmann transport theory. The optical properties absorption, optical conductivity, eloss, dielectric constants, reflectivity and refractive index were calculated for the energy range between 0 - 13.7 eV. Based on the ductile/brittle analysis, ZnSe identified as ductile material suitable for flexible wearable thermoelectric applications.

Keywords: DFT Study, Wien2k, II-VI Semiconductor, Band Structure, Mechanical Properties

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Introduction

Flexible thermoelectric materials and their devices have been receiving more attention because of their usages in wide areas, namely medicine, communication, health care, electronics and other areas. There is a demand to develop flexible, emission free, sustainable power sources. Thermoelectric materials and their devices fulfil the above demands by their stable and direct power conversion from body heat. Specifically, flexible thermoelectric materials are identified as promising candidates for curved heat sources due to their easy contact with curved areas. Merely, the fabrication of flexible thermoelectric devices using ductile thermoelectric semiconductors is quite challenging due to the lack of good p-type ductile thermoelectric materials. Zinc blend chalcogenides namely zinc sulfide (ZnS), zinc selenide (ZnSe) and zinc telluride (ZnTe) are important II–VI compound semiconductors [1-2] that have garnered significant interest due to their unique electronic, optical, and structural properties. Both materials

crystallize in the zinc blende structure and exhibit strong covalent–ionic bonding, contributing to their excellent stability with good ductile nature. ZnSe, with its wide bandgap, is particularly known for its transparency in the visible region and is commonly used in blue-green optoelectronic devices, laser diodes, and infrared optical components. ZnTe, on the other hand, has a somewhat narrower bandgap [3] and is favored for applications such as thin-film solar cells [4], radiation detectors, and heterojunction-based devices, where its excellent p-type conductivity plays a key role. To gain a deeper understanding of their properties at the atomic scale, first-principles calculations based on density functional theory (DFT) are increasingly used. DFT-based studies have been crucial in exploring the electronic band structures, charge distribution, mechanical properties, and optical response functions of these materials, aiding in the design and optimization of optoelectronic devices, solar cells, thermoelectric and other applications [5]. Hence, 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).

Numerous studies have explored both the experimental and theoretical aspects of ZnTe and ZnSe, providing valuable insights into their potential for various applications. Early investigations primarily focused on the electronic band structures and density of states (DOS) of both materials, revealing key details about their semiconductor behavior and optical transitions. Cardona [6] and Venghaus [7] are showed experimentally that ZnSe have direct energy band gap of 4.3 eV and 2.82 at room temperature respectively. Some theoretical studies have been conducted on ZnSe and ZnTe. Adetunji et al. [8] presented to ZnSe reveal a 2.72 eV band gap, split peaks in the density of states at −2 eV and between 8–11 eV. Perin et al., [9] 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. Laim et al., [10] investigated wurtzite ZnX (X = S, Se, Te) alloys were studied using FP-LAPW and mBJ potential, with direct band gaps of 3.672 eV, 2.722 eV, and 2.270 eV. Ghaleb et al., [11] calculated ZnSe show good agreement with experiments, with band gaps of 1.33 eV (LDA) and 1.34 eV (GGA), and calculated absorption coefficients. 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. Erum et al. [13] 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. Singh et al., [14] presented vacuum thermal annealing improves the crystallinity of ZnTe thin films, increasing crystallite size and reducing the optical band gap from 1.37 to 0.91 eV. Sharme et al., [15] ZnSe thin films have a decreasing bandgap (from 2.7 eV to 1.92 eV) with increasing annealing temperature, maintaining p-type semiconducting properties. Despite extensive research on ZnTe and ZnSe, gaps remain in understanding their properties under varying conditions such as strain, doping, and defects. Additionally, the effect of phase transitions and annealing on their electronic and optical behaviors is not fully explored.

In the present study, we have reported the complete analysis of ZnSe 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 thermoefficiency for thermoelectric applications.

Computational Method

All the reported values have been calculated using Density Functional Theory [16] implemented as Wien2k [17] code with Full Potential Linearized Augmented Plane Wave (FP-LAPW) method. By solving Kohn-Sham equation based on first principles calculations, the analysis has been made on structure finding, dos and band structure plotting, elastic and mechanical properties calculations along with optical and thermoelectric properties. The structure of the material ZnSe has been optimized by PBE-GGA [18] (Perdew-Berke Ernzerhof - Generalized Gradient Approximation) and mBJ [19] (modified Becke-Johnson) exchange potential. The muffin-tin sphere radius for Zn is 2.42 and for Se is 2.15. The basis sets R_{MT} x 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 and BoltzTraP [20] code is used for thermoelectric properties calculations.

Results and Discussions

Structural Properties

The zinc blend ZnSe possesses cubic structure with a space group F-43m belonging to the space group number 216 shows in Figure 1a and the structural information are given Table 1. The ground state properties lattice constants, volume, bulk modulus, pressure derivative bulk modulus and total energy are determined by using Birch-Murnaghan equation of state shown in Table 2 and the volume optimization curve is shown in Figure 1b. The calculated lattice constant a_0 = 5.768 (A^0) and bulk modulus = 59.411 (GPa) are good agreement with reported values. The binary ZnSe is a semiconducting material with direct band gap of 1.061 eV (PBE-GGA) and 2.623 eV (mBJ) located at Γ symmetry point where valence band maximum (VBM) and conduction band minimum (CBM) are meet at same point.

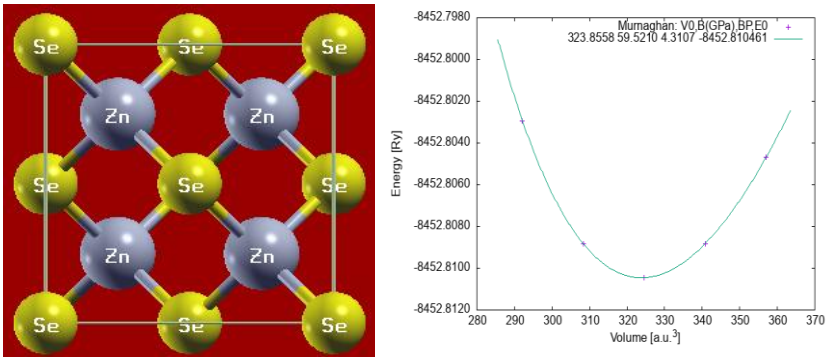


Figure 1. (a) Structure and (b) volume optimization curve of ZnSe

Table 1. Structural properties of ZnSe

Parameter/ Alloy	Atomic Position	Structure	Space group	No. of atoms in unit cell	E_g (eV)	NOE	E_F(Ry)
ZnSe	Zn (0.25,0.25,0.25) Se (0,0,0)	Cubic	216 - F-43m	2	1.061(GGA) 2.623(mBJ)	28	0.19667(GGA) 0.22442(mBJ)

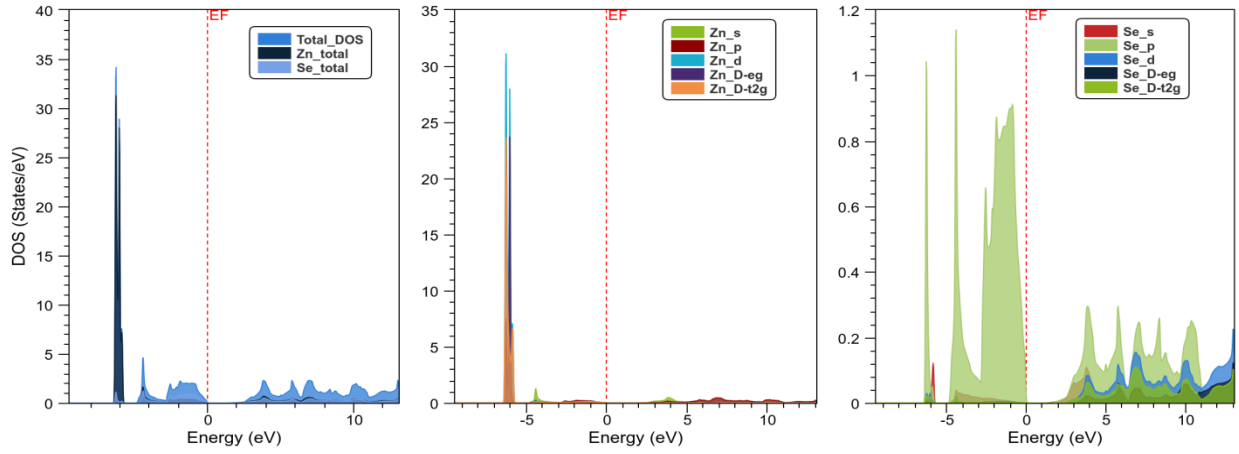
Table 2. Calculated lattice parameter a_0 (A^0), Volume (a.u.)^3, bulk modulus B(GPa), pressure derivative bulk modulus B' and total energy E_0 (Ry) for ZnSe

Parameter/ Alloy	a_0 (A^0)	V (a.u.)^3	B(GPa)	B'	E_0 (Ry)
ZnSe	5.768 5.773(exp) 5.728 [25] 5.578 [26]	323.856	59.41 58.50[25] 71.84[26]	4.30 3.94[25] 4.59[26]	-8452.810460

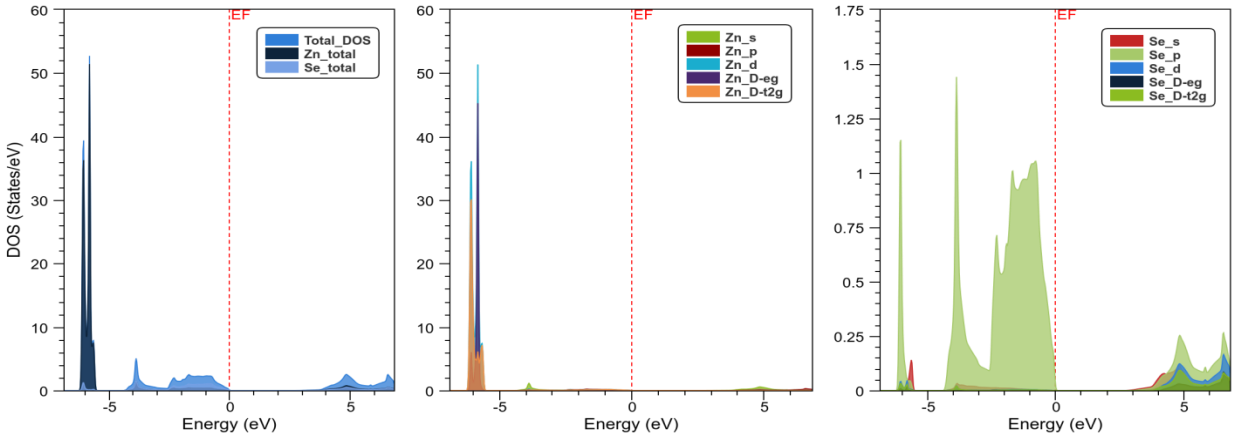
Electronic Properties

Density of States

The density of states histogram for ZnSe shown in Figure 2a (PBE-GGA) and Figure 2b (mBJ). In Figure 2a, it is clearly shown that below the fermi level is mainly due to Zn - d states and Se- s, p states; above the fermi level is mainly due to Zn - s, p states and Se-p states. There is a less contribution from Sn -s states to the regions in above the fermi energy level. The sharp peak below the fermi level is observed at -6.0 eV. The physical properties of the materials are changed by sharp peak, here it is governed by Zn - d states.



(a)



(b)

Figure 2. Total and partial density of states of ZnSe a) PBE-GGA b) mbj

Band Structure

The computed electronic band structure for ZnSe shown in Figure 3a(PBE-GGA) and Figure 3b(mBJ). The detailed analysis has been done by fat band structure of Zn and Se 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 -4.5 eV is mainly due to Zn - s, d, d-t2g states and Se -p states and little contribution from Zn - p, Se - s states

(iii) around -2.5 eV is mainly due to Zn - p and Se -p states; there is less contribution from Zn-d, d-t2g states

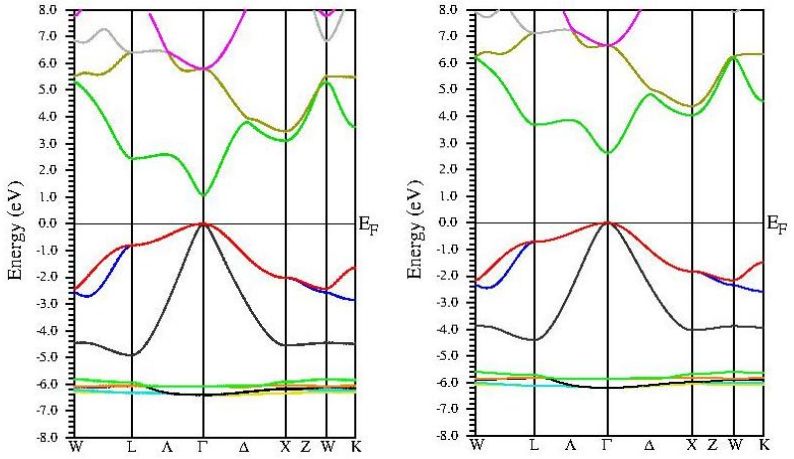
(iv) around -12 eV is mainly due to Se - s, p states

The top region above the fermi energy level -

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

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

From Figure 3b, it is clearly observed that increasing of band gap from 1.061 (GGA) to 2.623 eV (mBJ) is because of uplifting of Zn - s and Se- s, p states.



(a) (b)

Figure 3. Band structure of ZnSe a) PBE-GGA b) mbj

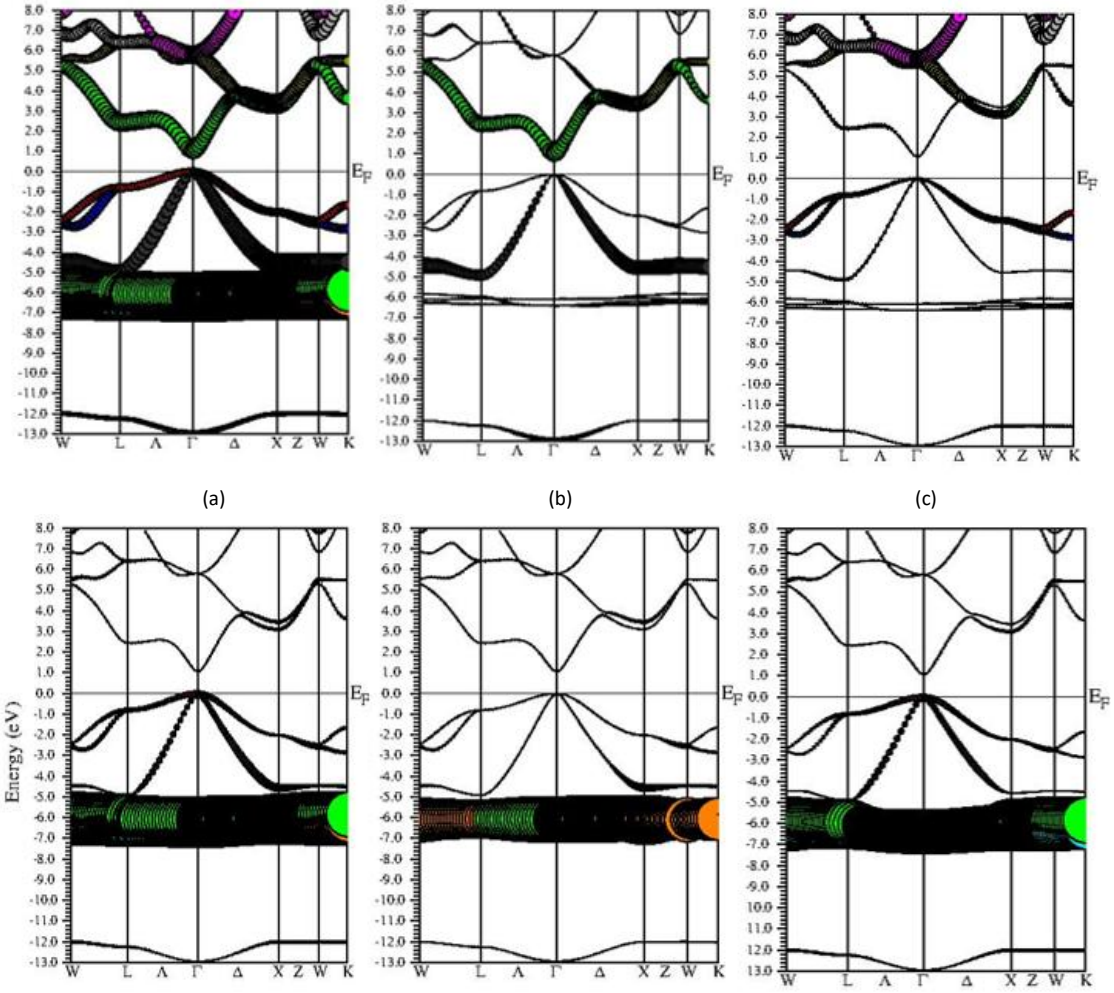
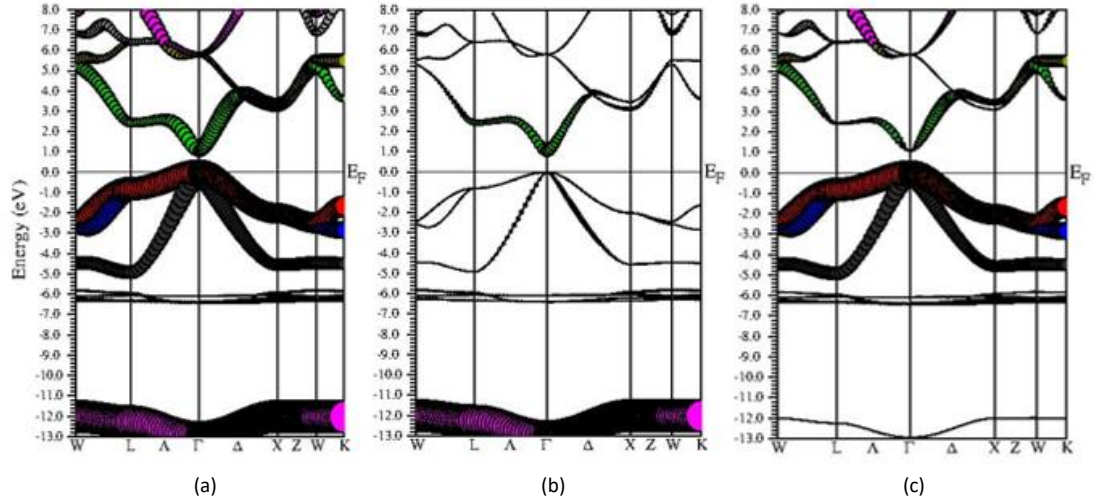
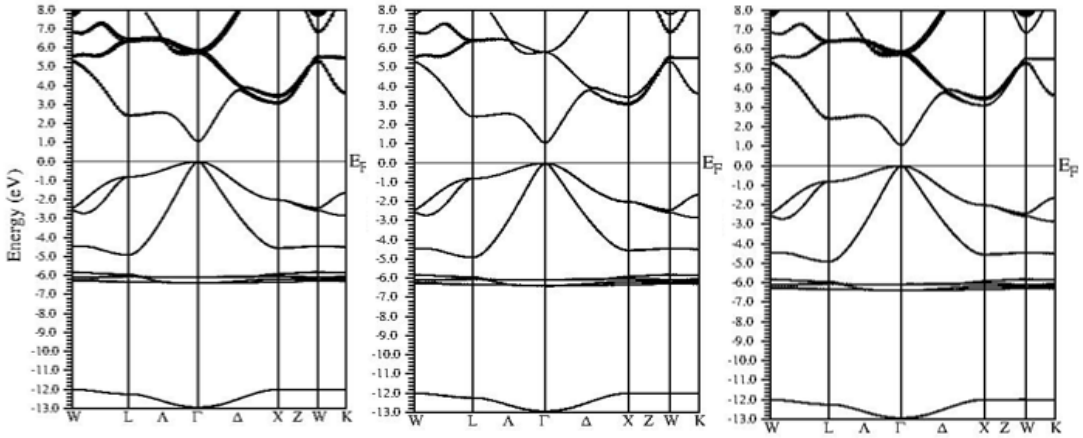


Figure 4. fat band structure of Zn a) total b) s- c) p- d) d- e) d-eg d) d-t2g states





(d) (e) (f)

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

Elastic, Mechanical and Thermal Properties

Elastic constants of inorganic materials are important physical properties of the crystal system to correlate the targeted mechanical responses. For a cubic crystal symmetry, three independent elastic constants namely C_{11}, C_{12} and C_{44} are required to calculate the mechanical properties [21]. We compute elastic constants C_{11}, C_{12} and C_{44} by Morteza Jamal method [22] for ZnSe 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 $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, $C_{11} > B > C_{12}$. 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 3. From the results, we identified ZnSe is a ductile material which is confirmed by the G/B ratio of 0.57 and positive Cauchy's pressure values also hardness becomes medium.

Further we have used these computed elastic constants to measure thermal properties of ZnSe material. Debye temperature (θ_D) has been calculated from average sound velocity $\mathbf{v}_m$ which is used to investigate the behaviour of the heat capacity of solids by the following equation

$$\theta_D = \left(\frac{h}{k_B}\right)\left[\frac{3n}{4\pi V_a}\right]^{\frac{1}{3}} V_m \qquad [1]$$

Here h is the Plank's constant, k_B Boltzmann's constant and V_a is the average atomic volume. The average wave velocity V_m and is calculated by the following equation,

$$V_m = \frac{1}{3}\left[\left(\frac{1}{{V_L}^3} - \frac{2}{{V_s}^3}\right)\right]^{-\frac{1}{3}} \qquad [2]$$

Here V_L and V_S are the sound velocities for longitudinal and shear elastic waves and given by the following equations

$$V_L = \sqrt{\frac{3B+4G}{3\rho}} \qquad [3]$$

and

$$V_S = \sqrt{\frac{G}{\rho}} \quad [4]$$

The anharmonicity of the materials can be calculated by the Grüneisen parameter (ξ) using the equation

$$\xi = \frac{9\left(V_L{}^2 - \frac{4}{3}V_S{}^2\right)}{2\left(V_L{}^2 + 2V_S{}^2\right)} \quad [5]$$

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 K GPa^{-1}) C_{11} ± 300 K [6]

From Table 4, we have noted lower Debye temperature, large Grüneisen parameter and maximum melting temperature, it indicates weak covalent nature of ZnSe material.

Table 3. Mechanical properties of ZnSe

	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	C_{12}-C_{44} (GPa)	B (GPa)	G (GPa)	E (GPa)	G/B	ν	H_v (GPa)
ZnSe	76.08 75.8[26]	43.15 48[26]	46.733 5.2[26]	-3.578	54.13 57.3 [26]	30.77 24.3 [26]	77.62 63.8[26]	0.57	0.3 0.31[26]	4.669

Table 4. Thermal properties of ZnSe

Parameter/ Alloy	V_L (m/s)	V_S (m/s)	V_m(m/s)	θ_D (K)	Tm(K)	ξ
ZnSe	4365	2482	2759	284	702	1.55

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), conductivity, absorption coefficient, optical energy loss function, reflectivity, refractive index and extinction coefficient are calculated using the GGA approximation and the results are analyzed and presented in Figure 6 (a-h).

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 13.7 eV as shown in Figure 6a & 6b. The real part attains maximum (10) at 3.2 eV and becomes negative (-2) at 5.6 eV. Optical conductivity can be calculated from the imaginary part of dielectric function and attains maximum optical conductivity value in the visible region at 5.5 eV. The maximum value of reflectivity reached the energy 8.2 eV. Energy loss becomes maximum at high photon energy.

Also we have noted that good optical absorption of the ZnSe with a wide energy range 0-13.7 eV and are potential material for optoelectronic devices in ultraviolet (UV) region. The maximum absorption coefficient was observed at 8.53 eV. The refractive index value lies between 0.15 to 2.8 with an energy range of 0 eV to 13.5eV. The maximum extinction coefficient value of 2.4 reached for ZnSe at the energy value of 5.3 eV.

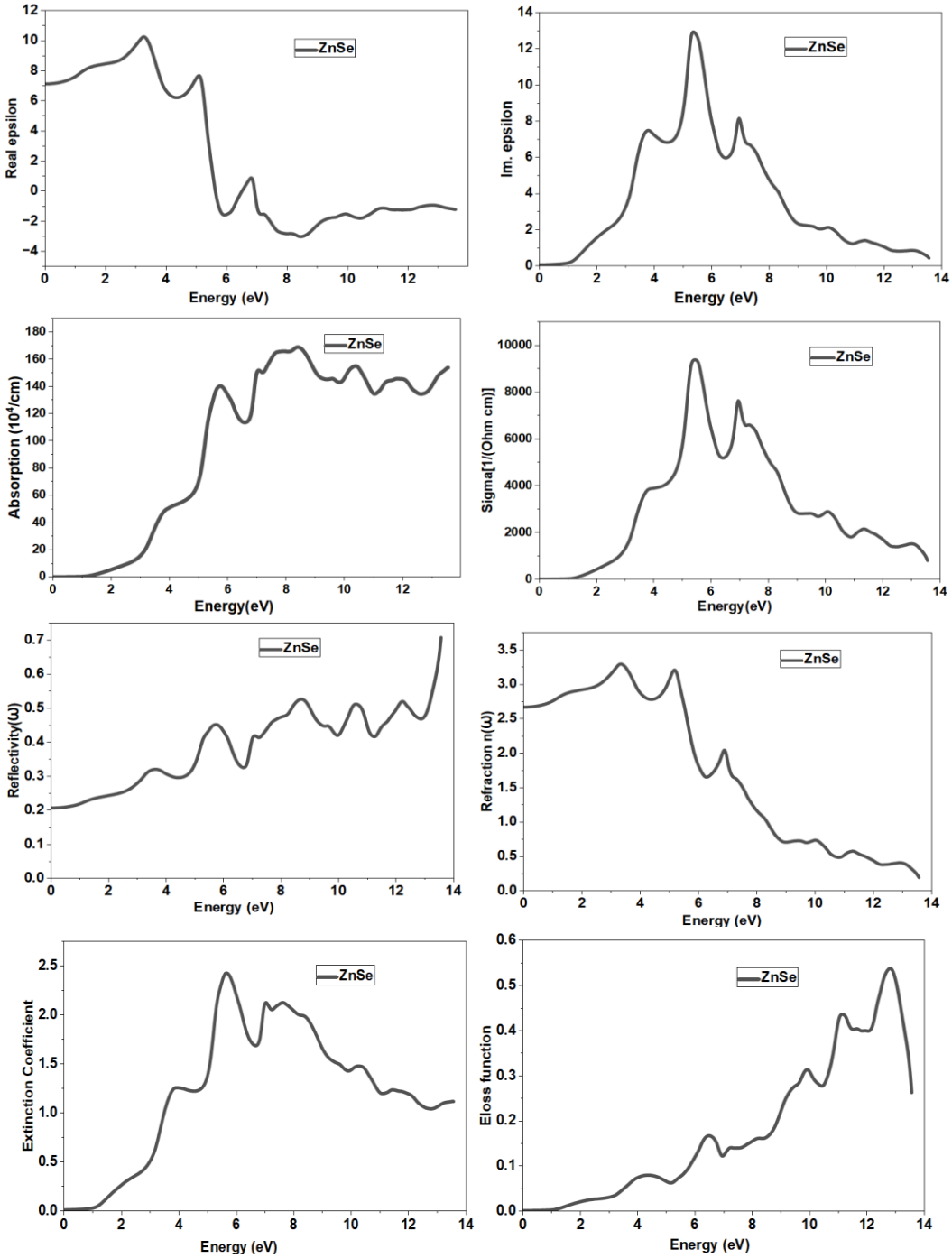


Figure 6. Optical properties of ZnSe

Thermoelectric properties

Thermoelectric properties of ZnSe 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,

$$ZT = \frac{S^2 \frac{\sigma}{\tau} T}{k_e + k_l} \quad [7]$$

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 5, the positive Seebeck value indicates that ZnSe is a p-type semi conducting material. From the results, ZnSe 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 5. Thermoelectric properties of ZnSe at 300 K for Fermi energy

Parameters	ZnSe
Seebeck Coefficient (S) (μV/K)	277
σ/τ x 10^{18} [1/(Ω m s)]	1.0677
$S^2 \sigma/\tau$ x 10^{16} [μW m^{-1} K^{-2} s^{-1}]	8.1923
Thermal Conductivity (κ^0) x 10^{12} [W/(m K s)]	7.2449
Electronic Specific Heat (c) [J/(mol K)]	0.0881
Hall Coefficient (R_H) x 10^{-7} [m^3/C]	1.3653
Pauli Magnetic (χ) x 10^{-13} [m^3/mol]	3.0677

Conclusions

In this work, the density function theory is employed to calculate structural, electronic, elastic, mechanical, optical and thermoelectric properties of zinc selenide using Wien2k code. From the detailed band structure analysis, we have identified the semiconducting nature of the ZnSe with direct band gap value E_g = 1.061 eV for GGA and 2.623 eV for mBJ potentials. 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 ZnSe identified as ductile material with less hardness. The optical responses of ZnSe calculated for the incident photon energy up to 13.7 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 ZnSe 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 = 277 (μV/K) indicates the ZnSe is a p-type

semiconducting material. The calculated power factor for ZnSe is 8.1923 ($\mu W\ m^{-1}\ K^{-2}\ s^{-1}$). From the study, it is concluded that the studied ZnSe material is a ductile p-type thermoelectric material which is a suitable candidate for flexible wearable thermoelectric applications. In future study, to find the series of ductile zinc blend chalcogenide thermoelectric materials by doping and co-doping method.

References

1. J. Liu, H. Liu, J. Wang, H. Sheng, G. Tang, J. Zhang, and D. Bai, "Optical and electronic properties of dichalcogenides WX2 (X = S, Se, and Te) monolayers under biaxial strain," *Physica B: Condensed Matter*, vol. 568, pp. 18-24, 2019. https://doi.org/10.1016/j.physb.2019.05.021
2. R. Mondal, Y.B. Singh, A.S. Das, S. Kabi, L.S. Singh, and D. Biswas, "Effect of Zn incorporation on physical properties of quaternary 0.7 Se–0.2 Ge–(0.1-x) Sb–xZn chalcogenide system: A theoretical prediction," *Physica B: Condensed Matter*, vol. 612, p. 412896, 2021. https://doi.org/10.1016/j.physb.2021.412896
3. M. Isik, H. H. Gullu, M. Parlak, and N. M. Gasanly, "Synthesis and temperature-tuned band gap characteristics of magnetron sputtered ZnTe thin films," *Physica B: Condensed Matter*, vol. 582, pp. 411968, 2020. https://doi.org/10.1016/j.physb.2019.411968
4. C. Nefzi, M. Souli, Y. Cuminal, and N. Kamoun-Turki, "Effect of substrate temperature on physical properties of Cu2FeSnS4 thin films for photocatalysis applications," *Materials Science and Engineering*: B, vol. 254, pp. 114509, 2020. https://doi.org/10.1016/j.mseb.2020.114509
5. F. Sarcan, M. Aydin, F. Kuruoğlu, O. Donmez, S. Yildirim, and A. Erol, "Temperature-dependent sandwich and in-plane optical characterization of ternary chalcogenide TlSbS2," *Materials Science and Engineering*: B, vol. 272, pp. 115322, 2021. https://doi.org/10.1016/j.mseb.2021.115322
6. M. Cardona, "Fundamental Reflectivity Spectrum of Semiconductors with Zinc-Blende Structure," *Journal of Applied Physics*, vol. 32, no. 10, pp. 2151-2155, 1961. https://doi.org/10.1063/1.1777034
7. H. Venghaus, "Valence-band parameters and g factors of cubic zinc selenide derived from free-exciton magnetoreflectance," *Physical Review B*, vol. 19, no. 6, p. 3071, 1979. https://doi.org/10.1103/PhysRevB.19.3071
8. B.I. Adetunji, P.O. Adebambo, and G.A. Adebayo, "First principles studies of band structure and electronic properties of ZnSe," *Journal of Alloys and Compounds*, vol. 513, pp. 294-299, 2012. https://doi.org/10.1016/j.jallcom.2011.10.039
9. G. Perin, D. Kuritza, R. Barbosa, G. Tresco, R.B. Pontes, R.H. Miwa, and J.E. Padilha, "First-principles study of bilayers ZnX and CdX (X = S, Se, Te) direct band-gap semiconductors and their van der Waals heterostructures," *Physical Review Materials*, vol. 7, no. 10, p. 104003, 2023. https://doi.org/10.1103/PhysRevMaterials.7.104003
10. I.A. Laim, A.S. Jbara, and H.K. Mohamad, "Structural, and electronic properties of ZnX (X = S, Se, Te) by first-principles calculation," in *AIP Conference Proceedings*, vol. 2398, no. 1, p. 020072, AIP Publishing LLC, 2022. https://doi.org/10.1063/5.0093962
11. A.M. Ghaleb, Y. B., A.Q. Ahmed, and Z. Talib, "Structural, electronic and optical properties investigation of ZnSe cubic sphalerite compounds using density functional theory (DFT),"

Problems of Atomic Science and Technology, vol. 1, no. 149, pp. 103-109, 2024. https://doi.org/10.46813/2024-149-103

12. B. Gul, M.M.A. Al-Hmoud, M.S. Khan, and S.M. Aziz, "A comparative DFT study of different structures of ZnTe: for optoelectronic and thermoelectric applications," *RSC Advances*, vol. 15, no. 20, pp. 15550-15560, 2025. https://doi.org/10.1039/D5RA01399B
13. N. Erum, Z. Ahmad, and M.K. Okla, "An ab-initio study of structural, opto-electronic and thermoelectric aspects of zinc sulfide and zinc telluride," *International Journal of Quantum Chemistry,* vol. 124, no. 1, p. e27293, 2024. https://doi.org/10.1002/qua.27293
14. H. Singh, N. Duklan, T. Singh, A. Thakur, and J. Sharma, "Effect of vacuum annealing on structural and optical properties of nanocrystalline ZnTe thin films," *Journal of Materials Science: Materials in Electronics*, vol. 29, no. 6, pp. 4992-4998, 2018. https://doi.org/10.1007/s10854-017-8460-7
15. Y. Sharma, P. Ansaria, R. Sharma, D. Mathur, and R. Dard, "Bandgap tuning of optical and electrical properties of zinc selenide," *Chalcogenide Letter*s, vol. 18, pp. 183-189, 2021. https://doi.org/10.15251/CL.2021.184.183
16. Hohenberg and W. Kohn, “Inhomogeneous Electron Gas” Phys. Rev. B, Vol. 136, 864, 1964. https://doi.org/10.1103/PhysRev.136.B864
17. P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, and J. Luitz, WIEN2k An Augmented Plane Wave Plus Local Orbitals Program for Calculating Crystal Properties (Vienna University of Technology, Vienna), 2008.
18. J. P. Perdew, S. Burke, and M. Ernzerhof, “ Generalized Gradient Approximation Made Simple”, Phys. Rev. Lett., vol. 77, pp. 3865, 1996. https://doi.org/10.1103/PhysRevLett.77.3865
19. F. Tran and P. Blaha, “Accurate Band Gaps of Semiconductors and Insulators with a Semilocal Exchange-Correlation Potential” Phys. Rev. Lett., vol.102, pp.226401, 2009. https://doi.org/10.1103/PhysRevLett.102.226401
20. M.Manjula, M.Muthumari and E.Viswanathan, "Thermoelectrics in alkaline earth metal tellurides of ATe2 type - A first-principles study", Physica Scripta, vol. 100, pp. 025925, 2025. https://doi.org/10.1088/1402-4896/ada591
21. M.Sundareswari, M.Manjula, D.Sivaprahasam and M. Muthumari, “Structure, electronic and thermoelectric properties of novel cubic Ir3V(1-x)Tix (x= 0.125, 0.25, 0.75, 0.875) refractory materials”, Computational Condensed Matter, vol. 39, pp. e00892, 2024. https://doi.org/10.1016/j.cocom.2024.e00892
22. M. Sundareswari, M. Manjula, D. Prabhu and D. Sivaprahasam, “Mechanical Properties of Ir3V1-xTix intermetallic Compounds”, Materials Letters, vol.358, pp. 135867, 2024. https://dx.doi.org/10.2139/ssrn.4656431
23. M. Muthumari, M.Manjula, Pandiyarasan Veluswamy and Denis Kuznetsov, “First principles calculations to investigate structural, electronic, mechanical, thermoelectric and optical properties of Bi-and Se-doped SnTe”, Journal of Physics and Chemistry of Solids, vol.176, pp. 111232, 2023. https://doi.org/10.1016/j.jpcs.2023.111232
24. M. Manjula, Pandiyarasan Veluswamy, Denis Kuznetsov, S. Krishnaveni and M. Muthumari, “Influence of ternary and quaternary inclusion on bandgap tuning of CaTe – Prediction of Potential Thermoelectric Materials. Journal of Electronic Materials, vol.50, pp. 1759 – 1771, 2021. https://doi.org/10.1007/s11664-020-08485-0

25. B.I. Adetunji a, P.O. Adebamboa, G.A. Adebayoa, “First principles studies of band structure and electronic properties of ZnSe” Journal of Alloys and Compounds, vol.513, pp. 294-299, 2012. https://doi.org/10.1016/j.jallcom.2011.10.039
26. TAN Jia-Jin, JI Guang-Fu,CHEN Xiang-Rong, “Phase Transition and Phonon Spectrum of Zinc-Blende Structure ZnX (X = S, Se,Te)” Communication Theoretical Physics, vol. 53, pp. 1160-1166, 2010. http://iopscience.iop.org/0253-6102/53/6/34