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# Structural and Optical Properties of ZnSe under Pressure

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***Abstract***

*The structural and optical properties of zinc selenide compound is investigated in zinc blende phases under 0-30 GPa pressure using density functional theory (DFT) calculations with generalized gradient approximation (GGA) embodied in Wien2k code. At zero pressure, lattice constant and bulk modulus are found to be in good agreement with experimental and other theoretical works. Other than zero pressure, there is a reduction in volume of the unit cell according to Murnaghan equation of state. The results of dielectric constant, refractive index, absorption coefficient and reflectivity versus (vs.) energy plots showed that the peak value increases as well as shift towards higher energies as we increase pressure. This increase or shift of peak values indicates the enhancement of direct band gap in ZnSe.*

***Keywords:*** *GGA, density functional theory, pressure dependent optical properties*

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## INTRODUCTION

Wide band gap materials like zinc selenide have vital applications for opto-electronic devices such as light emitting diodes (LEDs) and laser diodes (LDs). ZnSe exist in two crystalline forms: wurtzite (hexagonal) and zinc blende (cubic) of which the cubic phase is believed to be stable. The properties such as large bandgap, low resistivity and high photosensitivity make this semiconducting material highly attractive. Among different II–VI compound semiconductors, ZnSe has drawn considerable interest because of its direct and large band gap, which makes it appropriate for the fabrication of optical devices such as detectors as well as emitters [1–3].

Recently some researchers have reported their computational studies of the properties of ZnSe. Khanata and his fellows determined the structural and optical properties of ZnSe using first principle study. They determined lattice constant, elastic constant, bulk modulus, band structure, density of states and refractive indices [4]. Rusu GI studied ZnSe thin films experimentally using XRD techniques. They found that the structure was zinc blende (cubic). They also studied the spectral dependence of absorption coefficient in the range of 300–1400 nm [5]. Nourbakhsh Z, studied in detail the properties of ZnSe and also calculated their pressure dependent effects on structural, electronic and optical properties using Engel-Vosko approach within density functional theory by the Wien2k code. The main properties he calculated are energy band gap, real and imaginary parts of the dielectric function, energy loss function, optical absorption coefficient and reflectivity spectra. He investigated the effect of pressure on the energy band gap, the real and imaginary parts of the dielectric function [6]. Optical parameters like refraction, absorption, reflection, transmission, emission and scattering are energy dependent powerful tools for the understanding of the electronic nature of a material. In the present study, we have used GGA exchange and correlation potential to found the optical and structural properties under 0–30 GPa pressure first time, which might be useful for future study.

## COMPUTATIONAL DETAILS

We have used Wien 2k software, dealing with the structural properties and optical properties of ZnSe, which uses full potential linearized augmented plane wave plus local orbitals approach (FP-APW+lo) within generalized gradient approximation GGA. We determined the lattice type, lattice parameters and basis. We find the lattice type by simply viewing crystal shape as shown in Figure 1, and it is face centered cubic whose phase is zinc

 

blende. Using the optimization technique, we determined the lattice parameters. In this method, the volume of the ZnSe unit cell is changed against different values of total energy of every unit cell. As shown in volume optimization plot in Figure 1. We used the experimental value of lattice constant of ZnSe, which is 5.6676° Å to find out the theoretical value of lattice constant by using optimization method [1]. From Figure 1, the optimized volume $V_0$ against optimized energy 8450.928134 Ry is 301.5111 (a.u.$^3$). By using this formula, a= $[(V_0 * 4)^{1/3}]$ 0.52911706 we can calculate lattice constant which is 5.6321° Å in my case. We also get the value of bulk modulus B and optimized energy $E_0$, further we have determined the effects of applied pressure keeping the external applied pressure at 10 GPa, 20 GPa and 30 GPa.

In order to characterize the material optically we have found the complex relative dielectric constant, complex refractive index, absorption coefficient and reflectivity. The peaks on the graphs of dielectric constant, refractive index, reflectivity and absorption coefficient under applied pressure shows the behavior of these materials.

## RESULTS AND DISCUSSION

In order to analyze the effect of pressure on the lattice constant we used the following equation known as mornaghan equation of state $P(V) = \frac{B_o}{B'}\left[\left(\frac{V}{Vo}\right)^{-B'} - 1\right]$. Then using the method of optimizations by using first principle calculations in Wien2k code we calculated lattice constant and bulk modulus of both materials and further we have determined the effects of applied pressure keeping the external applied pressure at 10 GPa, 20 GPa and 30 GPa which revealed a significant decrease in the lattice constant. From the Table 1, we can see how the optimized energy is decreasing with the increase in pressure and also the volume of the unit cell is also decreasing and from the Figure 2 lattice constant decreases in length due to increase in pressure according to the Murnaghan equation of sate. The V/V◦ is greater than 90% and our values are comparable with the experimental values.

The real part of dielectric function, as all optical properties dependent on dielectric function, is shown in Figure 3. It is clear from Figure 3(a) that for energy 4 eV, sharp increase in $\varepsilon_1$ (ω) is observed in ZnSe and reaches at the peak on energy 5.5 eV. Then it starts to decrease with some variations and beyond 6 eV goes below zero. It reaches to the minimum at energy range of 6–7 eV and beyond 18 eV, it raises above zero and becomes constant. Increasing pressure also causes shift of peak towards higher energies. In case of ZnSe, $\varepsilon_1$ (0) the static dielectric constant approximately remains constant. And we can see our results in the Table 2.

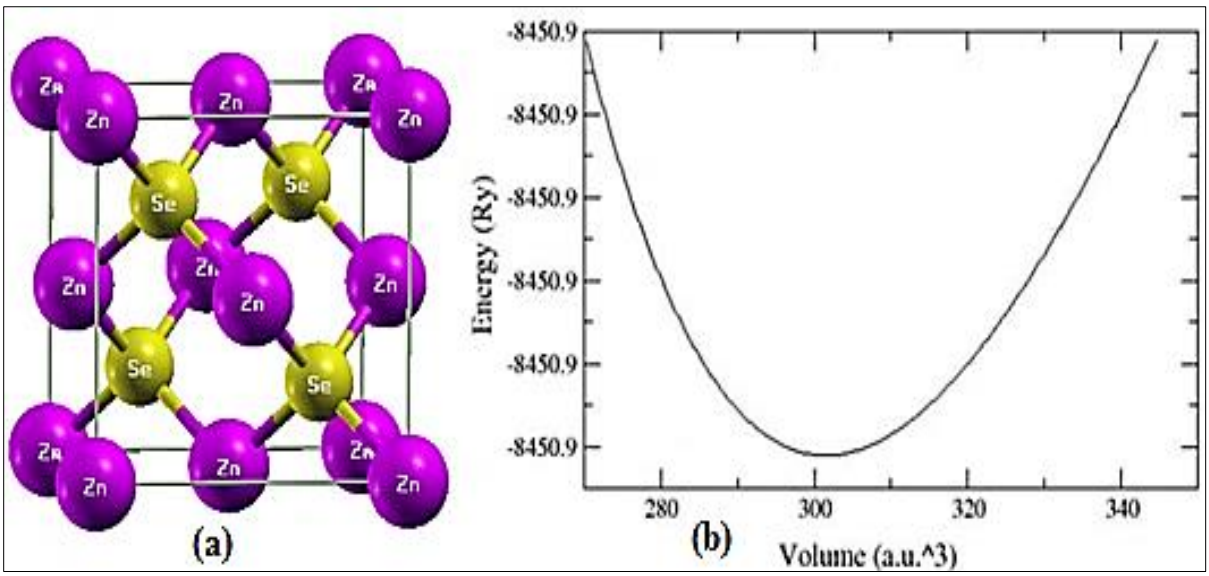


***Fig. 1:*** *Lattice and Optimization Graph.*

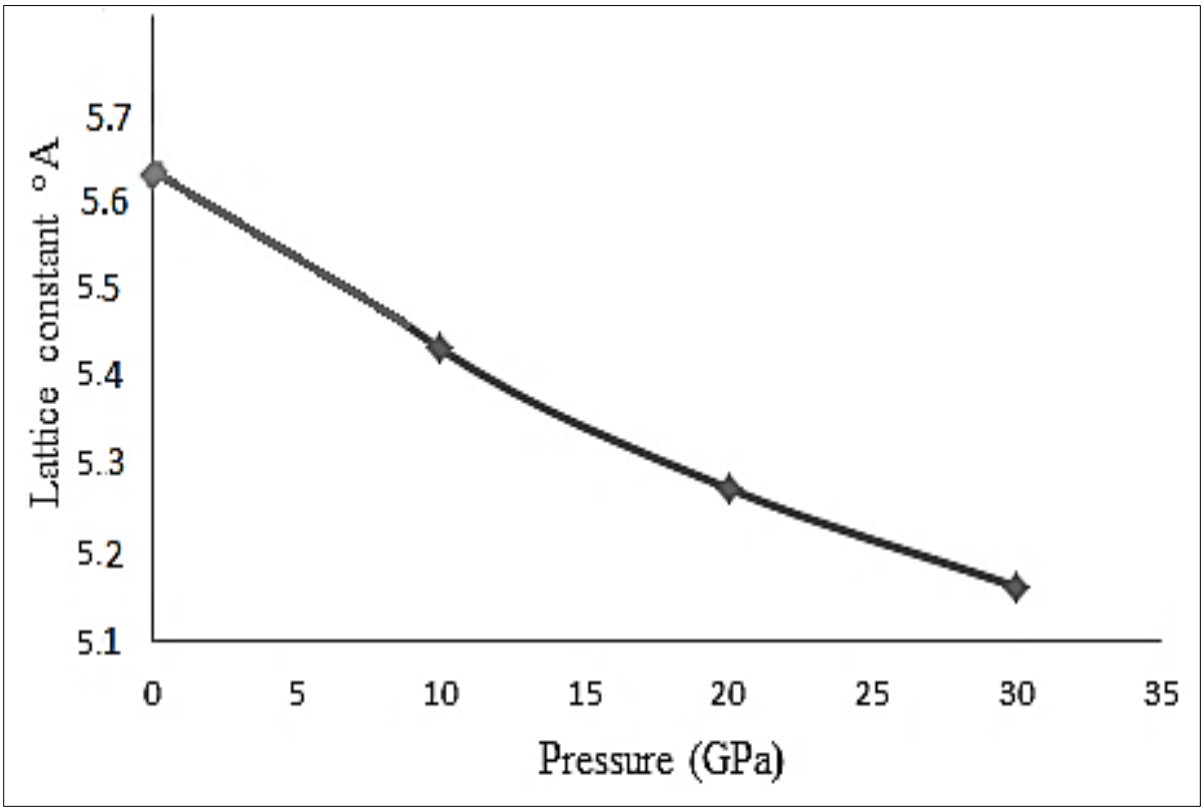


***Fig. 2:*** *Lattice Constant vs. Pressure Graph.*

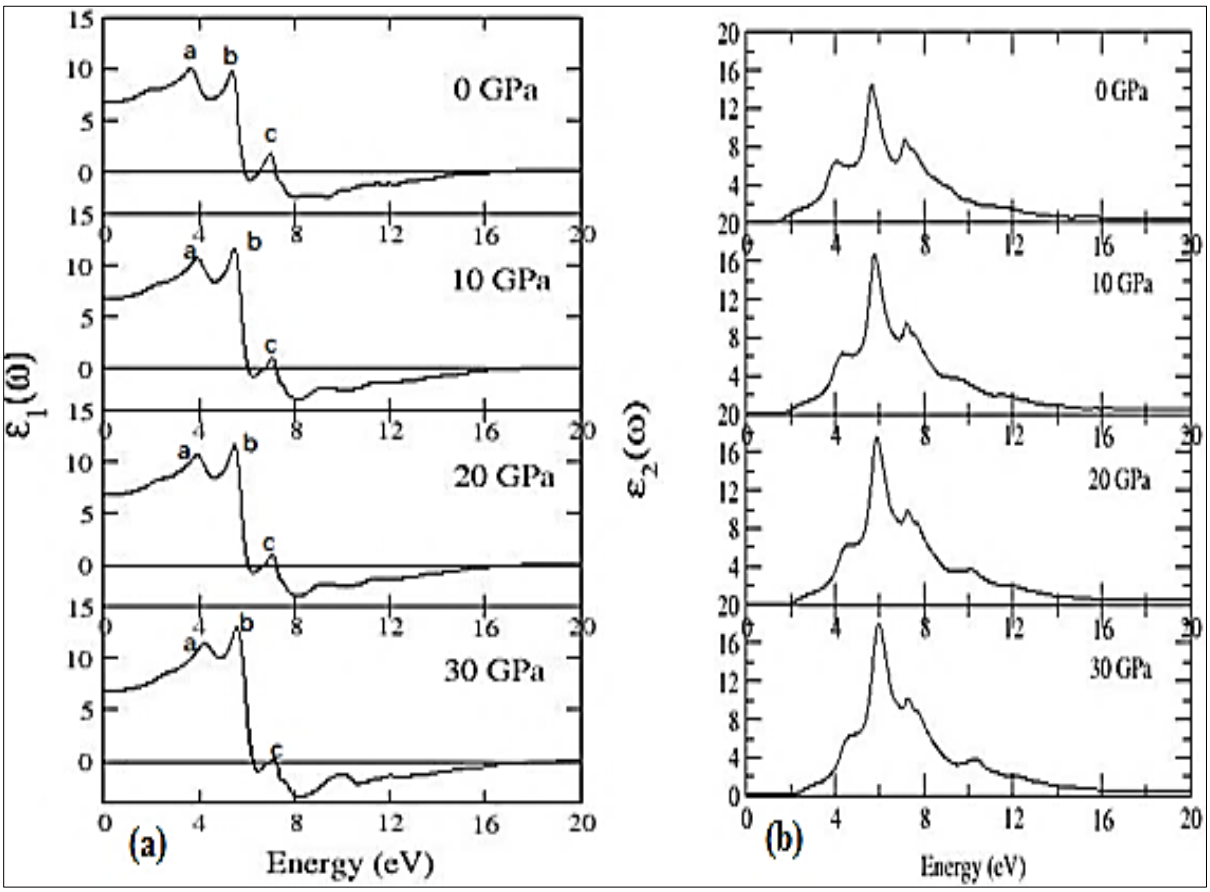


***Fig. 3:*** *$\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ vs. Energy Graph of ZnSe.*

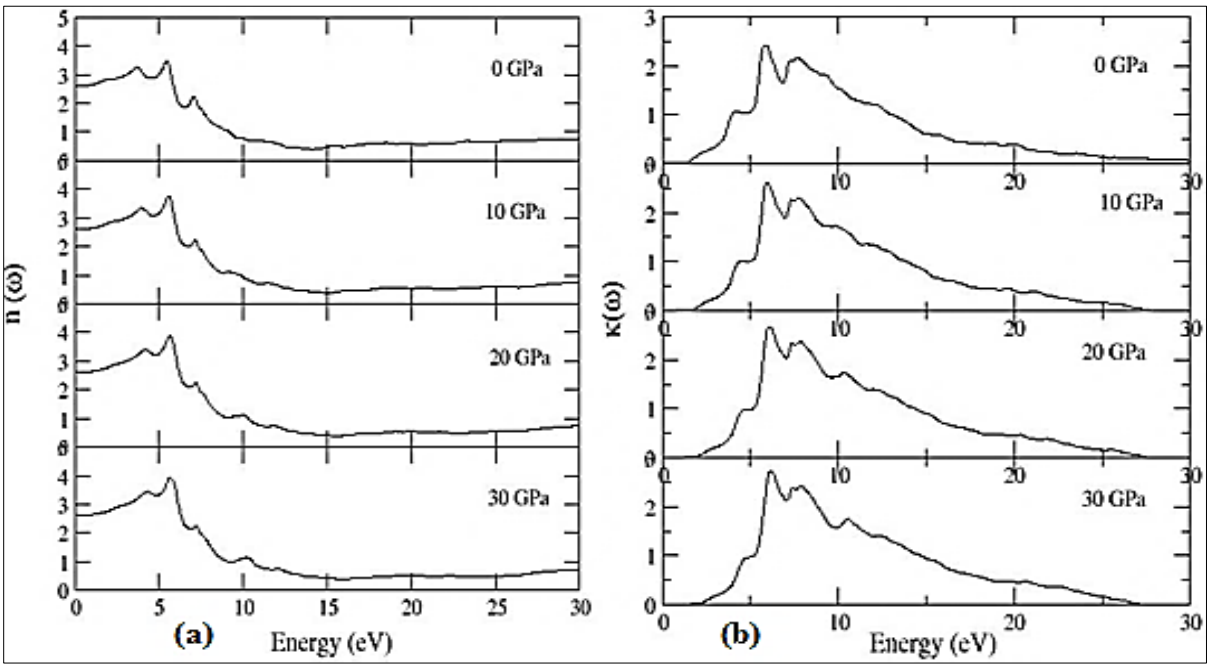


***Fig. 4:*** *n (ω) and κ (ω) vs. Energy Graph.*

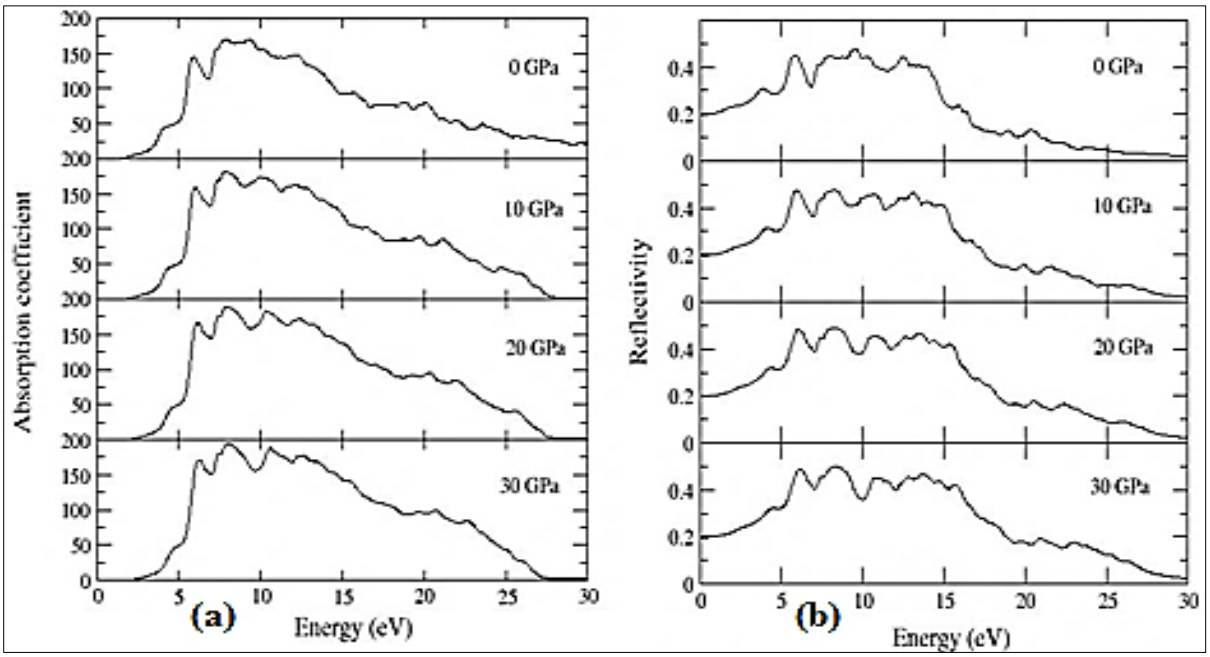


***Fig. 5:*** *Absorption Coefficient and Reflectivity vs. Energy Graph.*

From the Figure 3(a) and Table 2, we can easily see that the three peaks labeled as a, b, and c showing the behavior of ZnSe under ambient pressures and increasing towards higher values by increasing pressure. These peaks are also shifting towards higher energies under pressure because the direct band gap of ZnSe is increasing under pressure. From Table 2, the values of critical point and peak value of dielectric constant $\varepsilon_2(\omega)$ showing the similar pattern as the peak values are moving towards higher energy with increase in pressure. We observe similar pattern in the case of complex refractive index in which normal refractive index and extinction coefficient is increasing by increasing pressure from Figure 4, and also we can see this behavior in Table 3. From Figure 5(a, b) it is clear that the peak values in the graphs of absorption coefficient and reflectivity are increasing towards higher values which are shown in the Table 3.

***Table 1:*** *Effect of Pressure on Lattice Constant.*

| Pressure (GPa) | Volume, V (a.u.$^3$) | Optimized Energy, $E_o$ (Ry) | Lattice Constant, a ($^o$A) |
|---|---|---|---|
| 0 | 301.5111 | -8450.928134 | 5.6321 |
| 10 | 272.075 | -8450.876251 | 5.442 |
| 20 | 256.421 | -8450.871993 | 5.336 |
| 30 | 245.92 | -8450.868778 | 5.262 |

***Table 2:*** *Effect of Pressure on $\varepsilon_1(0)$, $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$.*

| Pressure (GPa) | Static Dielectric Constant $\varepsilon_1(0)$ | Dielectric Constant at Peak (b) value, $\varepsilon_1(\omega)$ | Critical Point (eV) | Dielectric Constant at Peak Value $\varepsilon_2(\omega)$ |
|---|---|---|---|---|
| 0 | 6.8 | 10 | 1.6 | 14.5 |
| 10 | 6.8 | 12 | 1.8 | 17 |
| 20 | 6.8 | 12.5 | 2 | 17.8 |
| 30 | 6.8 | 13.5 | 2.1 | 18.1 |

***Table 3:*** *Effect of Pressure on $n(\omega)$ and $\kappa(\omega)$ of ZnSe.*

| Pressure (GPa) | Normal Refractive Index at Peak Value n(ω) | Extinction Coefficient at Peak Value κ(ω) | Absorption Coefficient at Peak Value (α) | Reflectivity at Peak Value (R) |
|---|---|---|---|---|
| 0 | 3.5 | 2.4 | 165 | 0.47 |
| 10 | 3.7 | 2.6 | 175 | 0.48 |
| 20 | 3.8 | 2.65 | 185 | 0.49 |
| 30 | 4.0 | 2.75 | 195 | 0.52 |

## CONCLUSION

We investigated that the structural and optical properties of the ZnSe under 0–30 GPa pressure by performing full potential calculations within generalized gradient approximation (GGA) embodied in Wien2k code. Our result shows significant reduction in the lattice constant. The optical properties, real and imaginary parts of dielectric constant, refractive index, extinction coefficient, absorption coefficient and reflectivity, have also found at different pressure range. These results show that the peak values in graphs shift towards higher energies due to an increase in band gap values by increasing pressure.

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