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Pressure-Dependent Structural and Optical Properties of CdSe

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Abstract

The structural and optical properties of Cadmium Selenide (CdSe) compound is investigated in zinc blende phases under 0–30 GPa pressure using Density Functional Theory (DFT) with generalized gradient approximation (GGA) functional 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 reduction in volume of unit cell according to Murnaghan equation of state. The results of dielectric constant, refractive index, absorption coefficient and reflectivity versus energy plots showed that peak values increase as well as shift towards higher energies as we increase the pressure. This increase or shift of peak values indicates enhancement of direct band gap in CdSe.

Keywords: *Density functional theory, pressure-dependent optical properties, generalized gradient approximation (GGA)*

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INTRODUCTION

Wide band gap materials such as Cadmium Selenide (II–VI semiconductors) have vital applications for optoelectronic devices such as light emitting diodes (LEDs) and laser diodes (LDs). It converts to the wurtzite phase after heating and at very high pressure, it is converted into rock salt phase [1]. It is of great interest for its applications as high efficiency thin film transistors, solar cells, photoconductors, gas sensors, acoustic and optical devices, and photographic photoreceptors [2–9]. Major attention has been given in recent years to investigate the electrical and optical properties of CdSe thin films in order to improve the performance of the devices and also for finding new applications [10].

Khanata and co-workers determined the structural and optical properties of CdSe using first principle study with local density approximation (LDA) function. Their structural and optical properties showed it as a good material for optoelectronic devices [11]. Nourbakhsh studied first time optical and structural properties of CdSe under pressure using density functional theory (DFT) in Wien2k code. He investigated the effect of pressure in the range of 10–20 GPa [12].

In this article, optical parameters such as refraction, absorption, reflection, transmission, emission and scattering are energy-dependent powerful tools for the understanding of electronic nature of a material. In the present study, we have used generalized gradient approximation (GGA) exchange and correlation potential to find the optical and structural properties under 0–30 GPa pressure first time which might be useful for future study.

COMPUTATIONAL DETAILS

The phase of CdSe unit cell is zinc blende in face centered cube. The basis of our compound was two atoms per lattice point as shown in Figure 1(a). We used the full potential linearized augmented plane wave plus local orbital (APW+lo) method within GGA. In order to determine the lattice parameters in ground state, we calculated the total energy as a function of the unit cell volume in zinc blende phase. We used the optimization technique to obtain the optimized energy and at this energy the volume of unit cell V_0 was determined. From this volume, we calculated the lattice constant of the unit cell. The graph of volume optimization is shown in Figure 1(b).

From Figure 1(b), the optimized volume V_0 against optimized energy -8450.907624 Ry was 382.3146 (a.u.^{3}). By using a= $[(V_0 * 4)^{1/3}]$ 0.52911706, we calculated the lattice constant which was 6.096 Å in the present case. We also got the value of Bulk modulus B and optimized energy E_0. In our study, the lattice constant of CdSe was found as 6.096 ^{0}A which was very close to the experimentally found lattice constant 6.052 [13].

In order to characterize the material optically, we have found the complex relative dielectric constant, complex refractive index, absorption coefficient, and reflectivity. Theoretically we used Wien2k code to explore these properties and we have not only found the optical properties at ambient pressure but also we calculated the optical properties at increased pressures of up to 30 GPa. 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 Murnaghan equation of state:

$$P(V) = \frac{B_o}{B'}\left[\left(\frac{V}{Vo}\right)^{-B'} - 1\right] \quad (1)$$

Then using the method of optimizations by using first principle calculations in Wien2k code, we calculated lattice constant and Bulk modulus of both the 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 Table 1, we can determine the behavior of lattice constant which is decreasing according to the Murnaghan equation of state. The V/V_o was greater than 90% and our values were comparable with the experimental values. In order to investigate the optical properties, we considered only the cubic phase of CdSe. Because of the cubic symmetry of CdSe, we calculated only one dielectric tensor component to investigate the linear optical properties. We have found energy-dependent real and imaginary parts of the dielectric function for CdSe within GGA, using the equilibrium lattice constant. The real part of dielectric function is shown in Figure 2(a) and it is clear from the figure that for energy 3 eV, sharp increase in $\varepsilon_1(\omega)$ was observed in CdSe and reached at the peak after energy 5.5 eV.

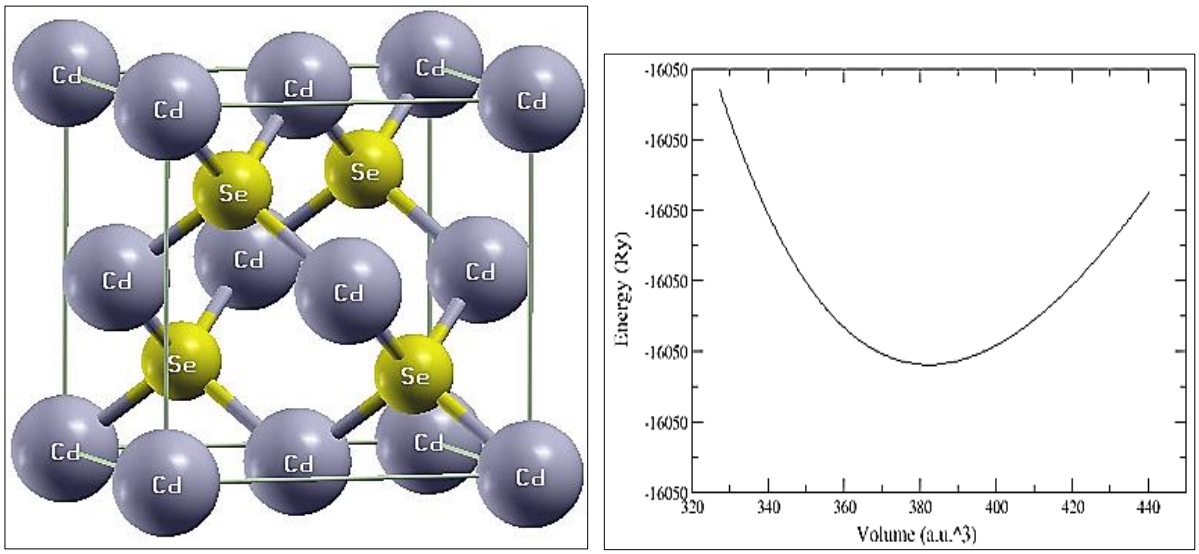

Fig. 1: *Lattice Structure and Optimization Graph of CdSe.*

Then it starts to decrease with some variations and beyond 6.5 eV goes below zero. These peaks shift towards higher energies by increasing pressure. Similarly the peaks in the graph of $\varepsilon_2(\omega)$, as shown in Figure 2(b), also shift towards higher energies by increasing pressure on CdSe. From Table 2, we can observe that the peak value goes up to 13 from 8.5.

We have determined the refractive index—one of the important optical properties—within GGA. From Table 3, we can observe that normal refractive index is increasing by increasing pressure and also we can observe the behavior of the graph in Figure 3(a). Extinction coefficient of CdSe under pressure was showing its behavior which is very clear from Figure 3(b) as we can see that the peaks of the graph shift towards higher values as we increase the pressure values. The same kind of behavior can be observed in the case of absorption coefficient *I (ω)* and reflectivity *R (ω)* in Figure 4(a, b), which also have been calculated within GGA. Table 3 shows the peak values of (α) and R increasing as we are increasing the pressure.

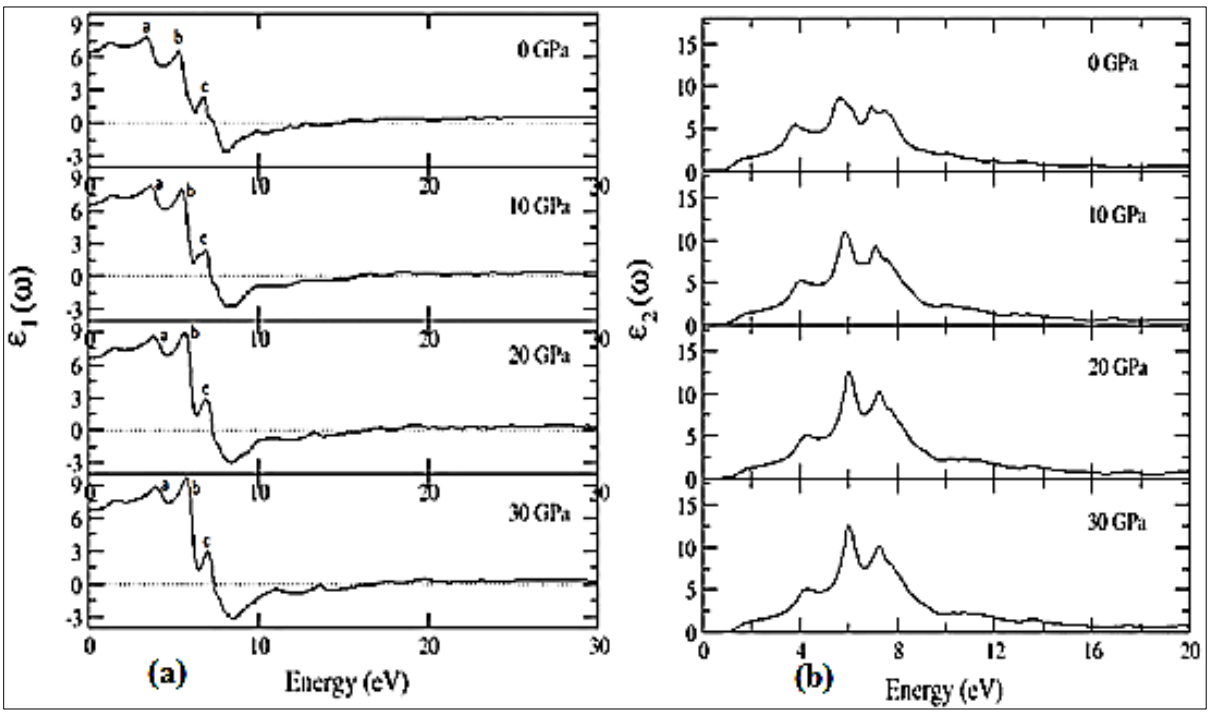

Fig. 2: *$\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ Versus Energy Graph of CdSe.*

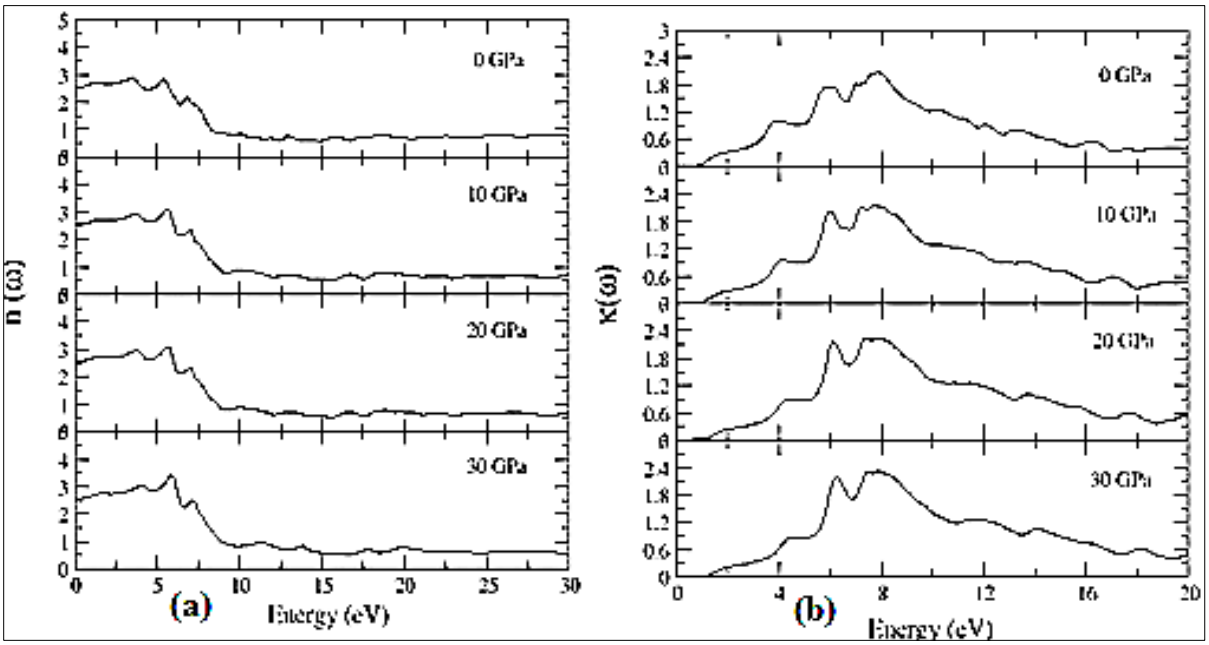

Fig. 3: *n (ω) and κ (ω) Versus Energy Graph.*

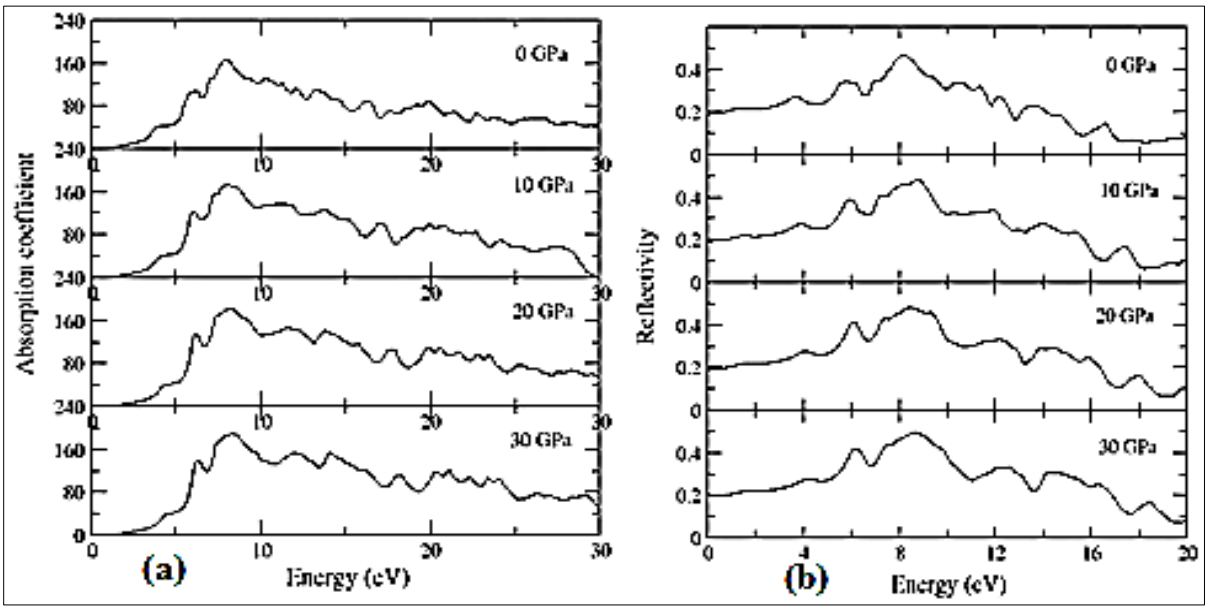

Fig. 4: *Absorption Coefficient and Reflectivity versus Energy Graph.*

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

Pressure (GPa)	Volume, V (a.u.^{3})	Optimized energy, E_o (Ry)	Lattice constant, a (Å)
0	382.3146	–8450.907624	6.096
10	334.13	–8450.887429	5.828
20	307.98	–8450.883477	5.672
30	290.46	–8450.879786	5.562

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	6.2	7.8	0.9	8.5
10	6.9	8.5	1	11
20	6.9	9.0	1.1	12.5
30	6.9	10	1.2	13

Table 3: *Effect of Pressure on n (ω) and κ (ω) of CdSe.*

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	3.0	2.4	170	0.47
10	3.1	2.6	175	0.49
20	3.2	2.65	180	0.49
30	3.3	2.75	190	0.50

CONCLUSION

We investigated the structural and optical properties of CdSe under 0–30 GPa pressure using DFT within GGA functional embodied in Wien2k code. Our results showed significant reduction in the lattice constant. The optical properties, real and imaginary parts of dielectric constant, refractive index, extinction coefficient, absorption coefficient and reflectivity, were also found at different pressure range. The results of dielectric constant, refractive index, absorption coefficient and reflectivity versus energy plots showed that peak values increase as well as shift towards higher energies as we increase the pressure. This increase or shift of peak values indicates an enhancement of direct band gap in CdSe.

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