

# High Pressure Band Structure, Metallization and Superconductivity of ZnSe and CdSe

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**Abstract** The high pressure band structure, density of states, metallization, structural phase transition and superconductivity of cubic zinc blende type zinc selenide (ZnSe) and cadmium selenide (CdSe) are investigated using the full potential linear muffin-tin orbital (FP-LMTO) method. The ground state properties and band gap values are compared with the experimental results. The equilibrium lattice constant, bulk modulus and its pressure derivative and the phase transition pressure at which the compounds undergo structural phase transition from ZnS to NaCl are predicted from the total energy calculations. The density of states at the Fermi level ( $N(E_F)$ ) gets enhanced after metallization, which leads to the superconductivity in ZnSe and CdSe. The superconducting transition temperatures ( $T_c$ ) of ZnSe and CdSe are obtained as a function of pressure for NaCl structure. ZnSe and CdSe come under the class of pressure induced superconductors. When pressure is increased  $T_c$  increases in both compounds. The dependence of  $T_c$  on electron - phonon mass enhancement factor  $\lambda$  shows that ZnSe and CdSe are electron-phonon-mediated superconductors.

**Keywords** Metallization, Superconductivity, Znse and Cdse, High Pressure

**Subject Classification:** 71, 71.15Fv, 61.50.Ks, 64.70.Kb, 74.62.Fj

## 1. Introduction

The physical properties of materials undergo a variety of changes when they are subjected to high pressure [1]. The increase of pressure means the significant decrease in volume, which results in the change of electronic states and crystal structure. With the development of high pressure experimental techniques, investigations on pressure-induced structural phase transition, semiconductor-metal transition and superconducting transition are getting the attention of all. In particular, there is a great interest in the pressure induced structural phase transition and metallization of the group

II-VI compounds ZnSe and CdSe. One of the most important characteristics of semiconductor, which distinguish it from the metals and insulators, is its energy band gap. This property determines among other things, the wavelength of light which it can absorb or emit. As a result of this, wide range of LEDs and Lasers can be constructed with the wide range of visible and infrared portion of the spectrum. Concentration of impurities or doping materials also play important role to control the electronic and optical properties of semiconductors [1].

Group II-VI compounds are a wide band gap semiconductors with a range of technological applications including electronic and electro-optic devices, catalysis, chemical sensors and conductive solar cell window layers [2,3]. Hence, to gain a fundamental understanding of the structural phase transition, metallization and superconductivity of ZnSe and CdSe, the electronic band structure studies of these materials are essential and this motivated the present investigation. The electronic configuration of Zn, Cd and Se are  $[Ar] 3d^{10} 4s^2$  ( $Z = 30$ ),  $[Kr] 4d^{10} 5s^2$  ( $Z = 48$ ) and  $[Ar] 3d^{10} 4s^2 4p^4$  ( $Z = 34$ ) respectively. The valence electronic configurations chosen in our calculation are  $3d^{10} 4s^2$  for Zn,  $4d^{10} 5s^2$  for Cd and  $4s^2 4p^4$  for Se. The band structures and density of states corresponding to various pressures are obtained using the full potential linear muffin-tin orbital (FP-LMTO) method [4]. The calculated total energies were fitted to the Murnaghan's equation of state (EOS) [3], to determine the phase transition pressure and other ground state properties. Generally selenide compounds (ZnSe and CdSe) crystallize in zinc blende structure (ZnS) [1, 5]. In our calculation we have chosen zinc blende structure as the normal pressure structure of these compounds. Subjecting ZnSe and CdSe to high pressure leads to pressure induced metallization, structural phase transition and superconducting transition.

The band gap value for ZnSe and CdSe were experimentally measured by Goni *et al* [6]. Theoretically numerous results on the band structure of ZnSe and CdSe exist [3,7-14]. Recently, Chunyuan *et al* [1] presented the electrical property and phase transition of CdSe under high pressure. Also Shchennikov *et al* [2] presented thermoelectric

properties and phase transitions of eleven II-VI semiconductors under pressure using Seebeck effect. There is no high pressure studies related to metallization and superconductivity in both ZnSe and CdSe. This motivated us to take up the present investigation of these compounds under high pressure. In this work, full potential linearized muffin tin orbital method (FP-LMTO) is employed to study the effect of pressure on the band structure of these compounds.

All solids would become superconductors under sufficiently high pressure<sup>[16]</sup>. The non-metallic compounds with ionic or covalent bonding also become metals and subsequently start superconducting under pressure. Experimentally it is found that, the ionic compound CsI is a metal under high pressure and as the pressure is increased, superconductivity sets in CsI<sup>[17]</sup>. These results lead us to expect superconductivity in other ionic and semiconducting compounds under high pressure; especially those compounds which have already become metals. Prior to metallization these compounds undergo structural phase transition from zinc blende to NaCl structure. We have analyzed the phenomena of metallization and superconductivity at high pressure (NaCl) structures of these materials. It is hoped that this analysis will enable us to make some general statement regarding the path to high  $T_c$  superconductivity in covalent compounds.

In Section 2, we give the details of the calculational procedure and electronic band structure corresponding to various pressures. The ground-state properties, structural phase transition, metallization and superconducting transition temperature  $T_c$  and its variation under pressure are discussed in Section 3. Concluding remarks are given in Section 4.

## 2. Band Structure and Density of States

### 2.1. Calculational Procedure

The electronic band structure calculations were performed for ZnSe and CdSe corresponding to different reduced volumes both in ZnS and NaCl structures, by the first-principle linear muffin-tin orbital (FP-LMTO) method. We have used FP-LMTO method with in generalized gradient approximation (GGA)<sup>[18]</sup>. We have used the exchange-correlation potential of Ceperley and Alder as parametrized by Perdew and Zunger [19]. We give here only the calculational details. The electronic configuration of Zn, Cd and Se are  $[\text{Ar}] 3d^{10} 4s^2$  ( $Z = 30$ ),  $[\text{Kr}] 4d^{10} 5s^2$  ( $Z = 48$ ) and  $[\text{Ar}] 3d^{10} 4s^2 4p^4$  ( $Z = 34$ ) respectively. The valence electronic configurations chosen in our calculation are  $3d^{10} 4s^2$  for Zn,  $4d^{10} 5s^2$  for Cd and  $4s^2 4p^4$  for Se. There are 18 valence electrons contributing to the valence bands [20]. The final energy convergence is within  $10^{-5}$  Ry. The calculated total energies were fitted to Murnaghan's equation of state (EOS) [21], to determine the pressure derivative of bulk modulus  $B_0'$ .

### 2.2. Band Structure and Density of States of Znse and Cdse under Pressure

The band structures and density of states of ZnSe and CdSe were computed for various reduced volumes ranging from  $V/V_0=1.0$  to 0.3 in steps of 0.05 (Figs.1 to 8). Even though we have obtained the band structure for  $V/V_0$  values from 1.0 to 0.3, we have presented here the band structures of ZnSe and CdSe along the symmetry directions  $\Gamma$ -X-W-L- $\Gamma$ -K corresponding to volume compressions  $V/V_0=1.0$  and  $V/V_0=0.686$  for ZnSe, and  $V/V_0=1.0$  and  $V/V_0=0.6313$  for CdSe only (Figs.1,3,5 and 7). The overall topology of the band structure of ZnSe and CdSe at  $V/V_0=1.0$  (Figs.1 and 5) is same as that of previous calculations<sup>[7]</sup>.

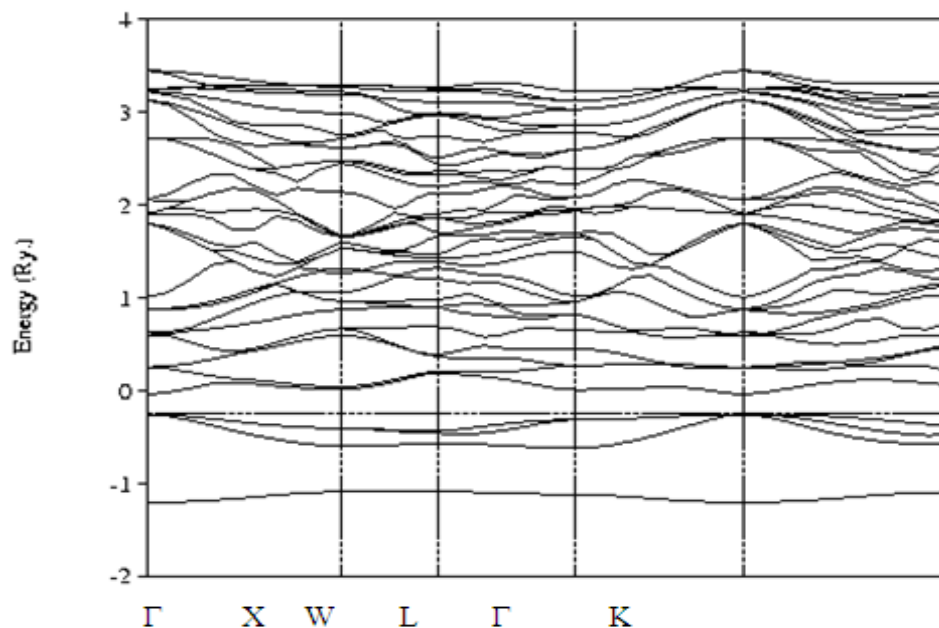


Figure 1. Band structure of ZnSe at normal pressure

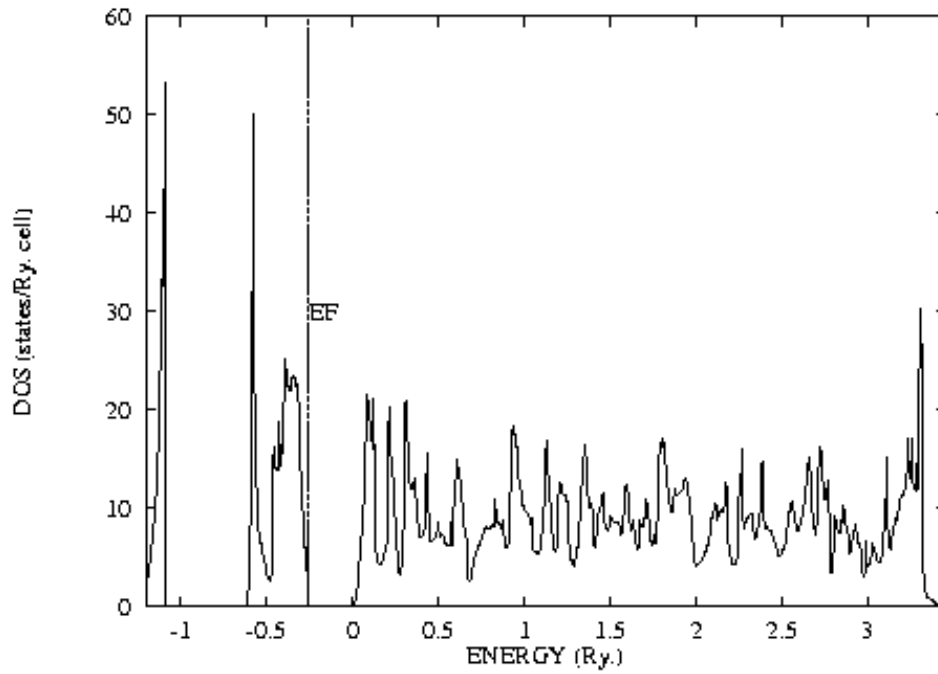


Figure 2. Density of states of ZnSe at normal pressure

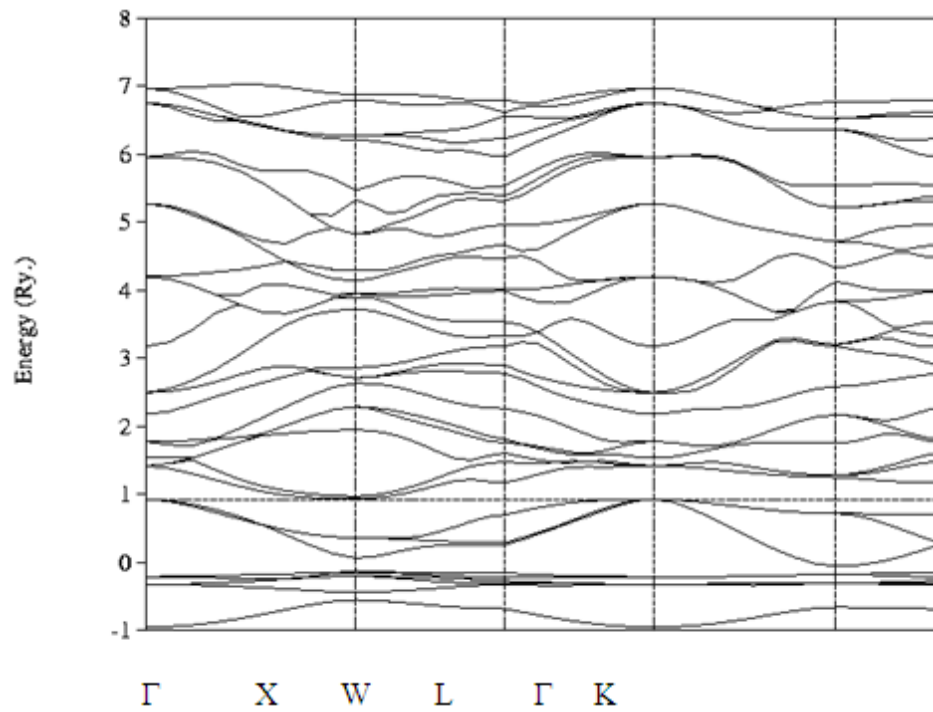


Figure 3. Band structure of ZnSe at metallization pressure

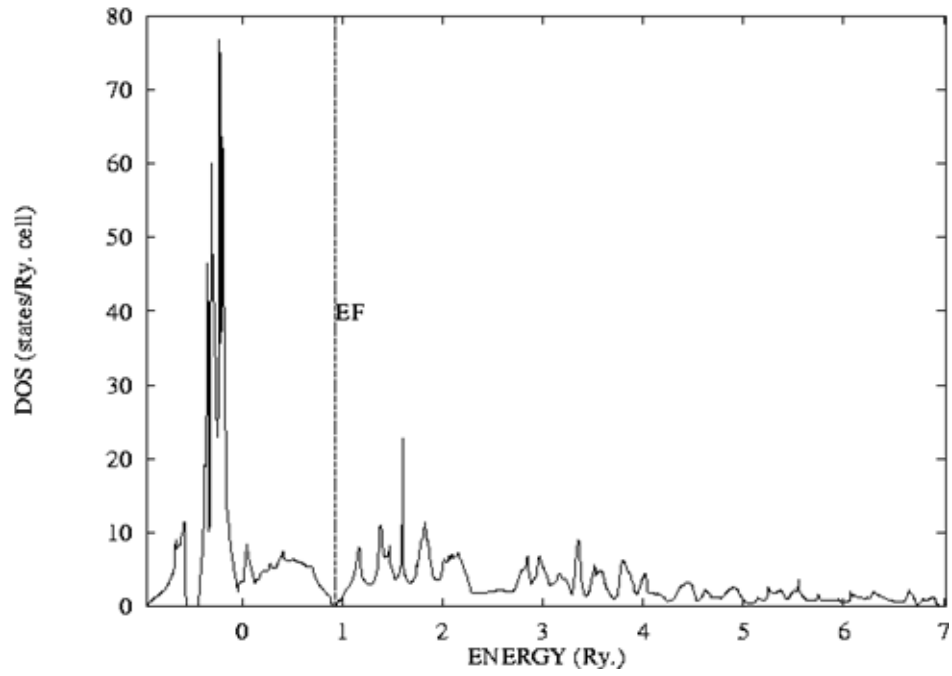


Figure 4. Density of states of ZnSe at metallization pressure

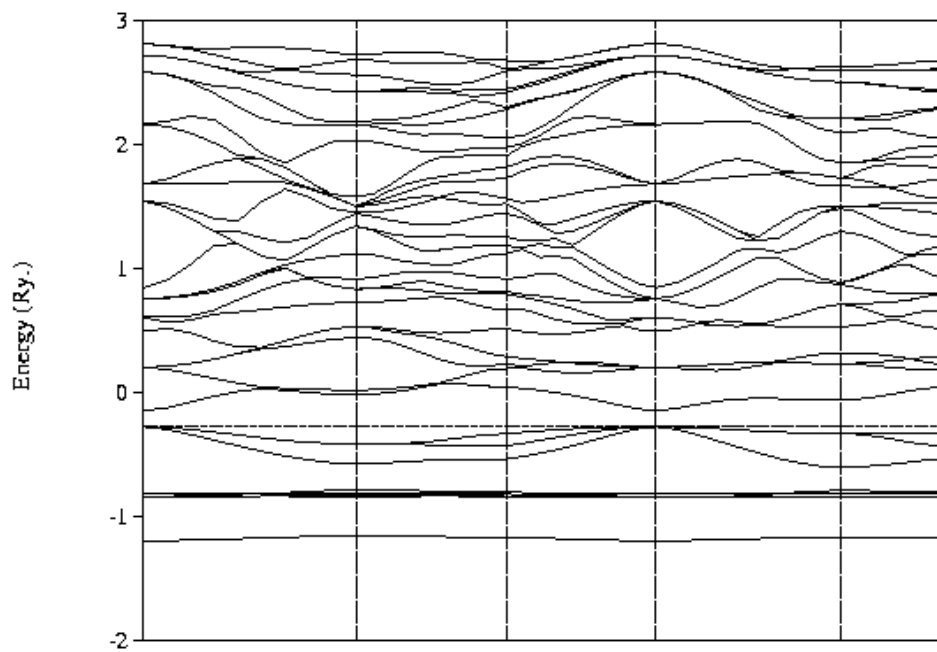


Figure 5. Band structure of CdSe at normal pressure

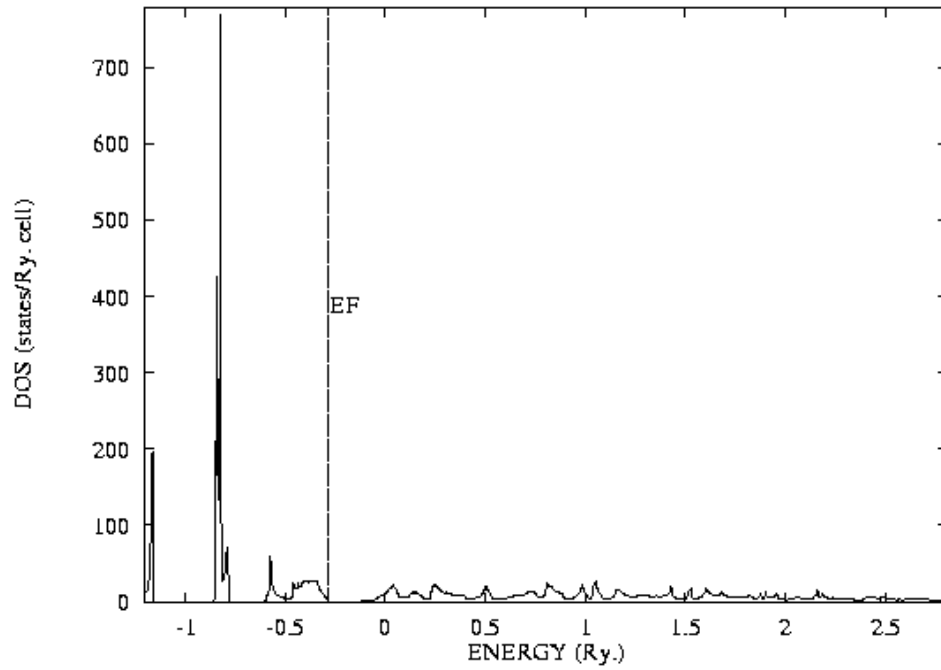


Figure 6. Density of states of CdSe at normal pressure

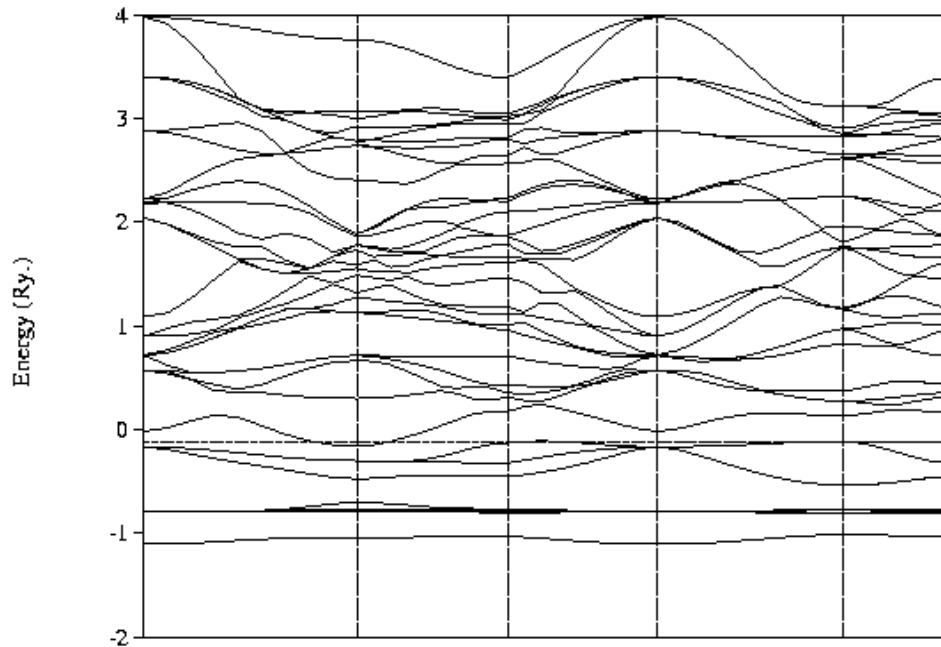
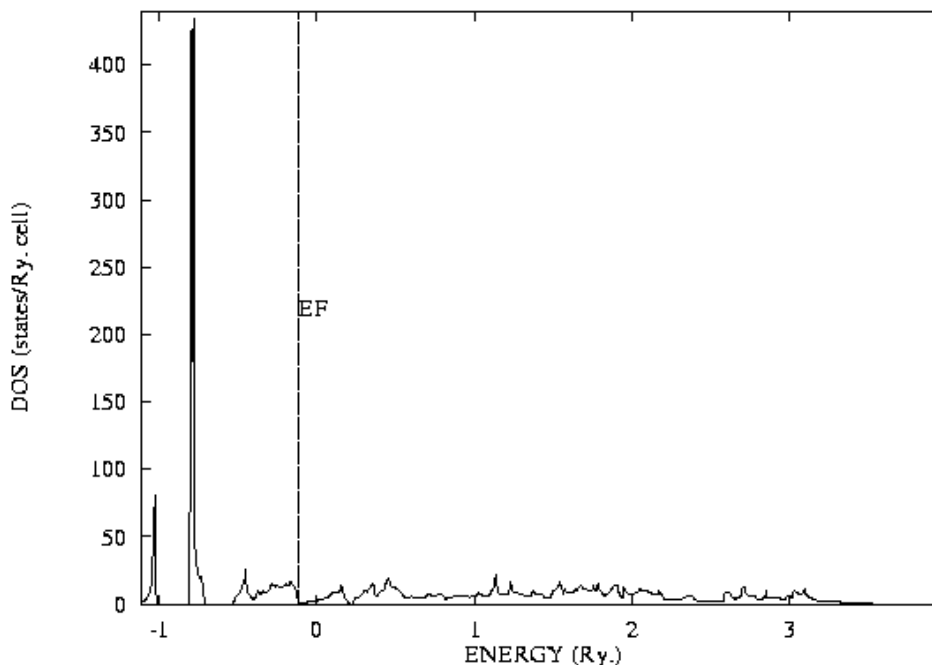


Figure 7. Band structure of CdSe at metallization pressure



**Figure 8.** Density of states of CdSe at metallization pressure

A single band which is positioned at the bottom of the valence band arise from  $4s^2$  electrons of Se (Figs.1 and 5). The three bands appearing below the Fermi level are due to the  $4s^2$  electrons of Zn and  $4p^4$  electrons of Se (Fig.1). The empty conduction bands above the Fermi level are due to  $4p$ ,  $4d$  states of Zn and  $4d$ ,  $5s$  states of Se (Fig.1). At normal pressure, the direct band gap is found to be 2.67 eV for ZnSe (at  $\Gamma$  point). In Fig.3, the five valence bands, which are positioned nearer to the  $4s$  bands arise from  $4d^{10}$  electrons of Cd (Fig.5). The three bands appearing below the Fermi level are due to the  $5s^2$  electrons of Cd and  $4p^4$  electrons of Se. The empty conduction bands above the Fermi level are due to  $5s$ ,  $4d$  states of Se and  $5d$ ,  $5p$  states of Cd (Fig.5). At normal pressure, the direct band gap is found to be 1.70 eV for CdSe (at  $\Gamma$  point). As pressure is increased, the increase in the width of the valence band and conduction band leads to the narrowing of the band gap and finally metallization in ZnSe at  $V/V_0=0.686$  ( $P_M = 0.709$  Mbar) (Fig.3) and CdSe at  $V/V_0=0.6313$  ( $P_M = 0.663$  Mbar) (Fig.7). Metallization occurs via indirect closing of band gap between  $\Gamma$  and X points (Figs.3 and 7). At the metallization pressure, there is appreciable value for density of states at Fermi energy  $N(E_F)$ . The values of  $E_F$  and  $N(E_F)$  are used in studying the pressure variation of superconducting transition temperature.

The density of states (DOS) (states/Ry.) calculations for all the reduced volumes has been carried out but here we have given the DOS histograms of ZnSe and CdTe corresponding to normal pressure (Figs.2 and 6) and metallization pressure (Figs.4 and 8). At normal pressure (Fig. 2) the levels arising from  $4s^2$  electrons of Se give the short spike near the origin. The long spike near the Fermi energy is due to  $4p^4$  and  $4s^2$  electrons of Se and Zn respectively. The short peaks above the Fermi energy  $E_F$  are

due to the  $4p$  and  $4d$  states of Zn and Se. As the pressure increases the width of the valence band and the empty conduction band get widened. These changes lead to the closing of the band gap under pressure (Fig.4). At normal pressure (Fig. 6) the levels arising from  $4s^2$  electrons of Se give the short spike near the origin. The longest spikes are due to  $4d^{10}$  electrons of Cd. The long spike near the Fermi energy is due to  $4p^4$  and  $5s^2$  electrons of Se and Cd respectively. The short peaks above the Fermi energy  $E_F$  are due to the  $4p$ ,  $4d,5p$  and  $5d$  states of Cd and Se. As the pressure increases the width of the valence band and the empty conduction band get widened. These changes lead to the closing of the band gap under pressure (Fig.8).

The general features of the band structure and density of states of ZnSe and CdSe are similar to that of the alkali halides <sup>[23]</sup>, but in ZnSe compound Zn –  $3d^{10}$  electrons not involved in the normal pressure band structure and density of states but at high pressure band structure and density of states it is involved. In CdSe compound Cd -  $4d^{10}$  electrons involved in the normal and high pressure band structure and density of states. These d electrons play an important role in the band structure <sup>[20]</sup>. The density of states histograms of ZnSe and CdSe at high pressure is given in Figs.4 and 8 respectively. At this pressure ZnSe and CdSe are in NaCl structure. From the histogram, it is seen that the heights of the spikes are considerably reduced when compared to Figs.6 and 8. Reason is when pressure increased  $E_F$  increases whereas no density of states is available at the Fermi level up to metallization pressure. There are appreciable values for DOS at  $V/V_0 = 0.686$  (Fig. 4) and  $V/V_0 = 0.6313$  (Fig. 8) indicating metallization in ZnSe and CdSe respectively <sup>[1]</sup>. When pressure increases (reduced volume decreases) the value of the DOS at Fermi energy,  $E_F$  ( $N(E_F)$ ) increases <sup>[2]</sup>.

The normal pressure DOS trend is changed under high pressure. The increase of pressure leads to the broadening of bands which results in the decrease of density of states value in most of the energy regions and also increases in the width of the valence band and empty conduction bands [24-32]. When pressure increases the value of  $E_F$  increases whereas no density of states is available at the Fermi level up to metallization pressure. Further increase in pressure leads to enhanced density of states at the Fermi level which induces superconductivity [20].

### 3. Results and Discussion

#### 3.1. Ground State Properties

The ground state properties and structural phase transitions of ZnSe and CdSe are studied from their total energies obtained from our calculation. The total energy is calculated as a function of reduced volume ( $V/V_o$ ) for both ZnS and NaCl phases of ZnSe and CdSe. Here,  $V_o$  is the experimental equilibrium volume corresponding to the experimental equilibrium lattice constant. The calculated total energies were fitted to Murnaghan's equation of state [21]

$$P = 1.5B_o \left[ \left( \frac{V_o}{V} \right)^{7/3} - \left( \frac{V_o}{V} \right)^{5/3} \right] \left[ 1 + 0.75 \left( B_o^{-1} - 4 \right) \left\{ \left( \frac{V_o}{V} \right)^{2/3} - 1 \right\} \right] \quad (1)$$

to obtain the pressure derivative of bulk modulus  $B_o'$  [23]. From the variation in the total energy as a function of reduced volume for ZnSe and CdSe, it is found that, in ZnSe, up to  $V/V_o = 0.942$  ( $P_T = 0.1160$  Mbar) and in CdSe, up to  $V/V_o = 0.967$  ( $P_T = 0.0312$  Mbar), ZnS structure has the lowest energy and on further reduction of volume NaCl structure becomes more stable in energy than the ZnS structure. In Table 1, the equilibrium lattice constant ( $a_o$ ), band gap ( $E_g$ ), bulk modulus ( $B_o$ ) and its pressure derivative ( $B_o'$ ) values are compared with experimental and previous theoretical works [1-7]. From Table 1, it is observed that one gets larger lattice constant corresponding to smaller bulk modulus. Our estimated bulk modulus of CdSe is less than that of ZnSe, as a result compressibility is higher for CdSe than ZnSe. Thus, it is noted that the compressibility decreases as the size of the cation decreases. This is the general trend in alkali halides [23], which is confirmed now for ZnSe and CdSe.

#### 3.2. Structural Phase Transition

In our calculation we have chosen the ZnS structure for both ZnSe and CdSe at ambient pressure. The phase stability of the B3 (ZnS) and B1 (NaCl) structures of ZnSe and CdSe is analysed using the enthalpy calculation [23]. The enthalpy  $H(P)$  is defined by

$$H(P) = E_{\text{tot}}(P) + PV(P) \quad (2)$$

and the transition pressure corresponding to the phase transition from B3 to B1 is obtained from the relation

$$H_{B3}(P) = H_{B1}(P) \quad (3)$$

where  $H_{B3}$  and  $H_{B1}$  are the enthalpies of the B3 and B1 phases respectively. From the enthalpy calculation, the phase transition pressure ( $P_T = 0.1160$  Mbar) and the corresponding reduced volume ( $(V/V_o)_T = 0.942$ ) are estimated for ZnSe and the phase transition pressure ( $P_T = 0.0312$  Mbar) and the corresponding reduced volume ( $(V/V_o)_T = 0.967$ ) are estimated for CdSe (Table.2).

Our calculated phase transition pressure of ZnSe supports the experimental value of 0.125 Mbar [31]. In the case of CdSe, experimental value is 0.032 Mbar [32]. The mechanism for the phase transition is a geometric effect involving a change in the coordination number from 4 in the ZnS phase to 6 in the NaCl phase [20].

#### 3.3. Metallization

At normal pressure, ZnSe and CdSe are direct band gap semiconductors. With the increase of the pressure, the band gap decreases and at a particular pressure, there is a closing of the band gap. The band structure corresponding to metallization of ZnSe and CdSe are shown in Figs. 3 and 7 respectively. In ZnSe and CdSe, the metallization occurs through indirect closing of the band gap between  $\Gamma$  and  $X$  points (Figs.3 and 7). The metallization volume of ZnSe is  $V/V_o = 0.686$  (NaCl structure), which corresponds to the pressure  $P_M = 0.709$  Mbar. In the case of CdSe, the indirect closure of the band gap between  $\Gamma$  and  $X$  point takes place at the reduced volume  $V/V_o = 0.6313$  (NaCl structure), the corresponding metallization pressure is 0.663 Mbar (Fig.7). This value is in good agreement with the experimental value of 0.7 Mbar [1]. For ZnSe, no experimental metallization value available for comparison.

The metallization pressure calculated for ZnSe is greater than that of CdSe (Table 2). This means, in group II-VI compounds, metallization pressure increases with the decreasing size of the group - II element. This trend is similar to the trend observed in alkali halides having NaCl structure at ambient conditions (metallization pressure increases with decreasing size of alkali metal [23]). The reason for this similarity is that, prior to metallization, alkali halides undergo structural transition from NaCl to CsCl structure whereas group II-VI compounds undergo structural transition from ZnS to NaCl structure [7]. At the metallization pressures, the values for density of states at Fermi energy  $N(E_F)$  are very small, which indicate that metallization has just set in ZnSe and CdSe ( Figs. 4 and 8 respectively).

Thereafter  $N(E_F)$  increases slowly with pressure and becomes fairly large at a particular value of  $V/V_o$ . The values of  $E_F$  and  $N(E_F)$  corresponding to different  $V/V_o$  are used in studying the pressure variation of superconducting transition temperature [20]. However, there is no experimental or theoretical study available for comparison at these pressures.

**Table 1.** Equilibrium lattice constant ( $a_o$ ), bulk modulus ( $B_o$ ) and its pressure derivative ( $B_o'$ ) of ZnSe and CdSe in ZnS structure

Ground State Properties	ZnSe			CdSe		
	Present work	Experimental works	Previous theoretical works	Present work	Experimental works	Previous theoretical works
$a_o$ a.u.	10.681	10.695 [26]	10.421 [9] 10.432 [3]	11.441	11.455 [26]	11.127 [9] 11.133 [3] 11.24 [32]
$B_o$ Mbar	0.705	0.765 [26]	0.671 [9] 0.657 [3]	0.572	0.585 [26]	0.519 [9] 0.417 [3] 0.515 [27]
$B_o'$	5.201	5.53 [8]	4.657 [3]	4.681	4.697 [8]	4.543 [3]
$E_g$ eV	2.67	2.71 [6]	1.820 [7] 1.754 [3]	1.70	1.751	1.360 [7] 1.192 [3]

**Table 2.** Metallization, phase transition and superconducting transition pressures in ZnSe and CdSe

Gallium Compound	Metallization		Phase transition		Onset of superconducting transition	
	$P_M$ Mbar	$(V/V_o)_M$	$P_T$ Mbar	$(V/V_o)_T$	$P_S$ Mbar	$(V/V_o)_S$
ZnSe	0.709	0.6860	0.1160	0.942	1.5	0.475
CdSe	0.663	0.6313	0.0312	0.967	1.5	0.525

### 3.4. Superconductivity in ZnSe and CdSe under Pressure

The promotion of  $s$  electron to  $d$  shell in solids is one of the factors which will induce superconductivity. Under very high pressure, selenides compounds are not only metals but also superconductors. The theory of Gaspari and Gyorffy<sup>[33]</sup> in conjunction with McMillan's formula is used to calculate  $T_c$ .

The electron-phonon mass enhancement factor,  $\lambda$  is<sup>[33]</sup>

$$\lambda = \frac{N(E_F)\langle I^2 \rangle}{M\langle \omega^2 \rangle} \quad (4)$$

where  $M$  is the atomic mass,  $\langle \omega^2 \rangle$  is an average of the phonon frequency square and  $\langle I^2 \rangle$  is an average (over the Fermi energy) of the electron-phonon matrix element square<sup>[34]</sup>.  $\langle I^2 \rangle$  (in Rydbergs) can be written as

$$\langle I^2 \rangle = 2 \sum_l \frac{(l+1)}{(2l+1)(2l+3)} M_{l,l+1}^2 \frac{N_l(E_F)N_{l+1}(E_F)}{N(E_F)N(E_F)} \quad (5)$$

Where

$$M_{l,l+1} = -\phi_l \phi_{l+1} [(D_l(E_F)-1)(D_{l+1}(E_F)+1+2) + (E_F-V(S))S^2]$$

and in this,

$\phi_l$  is the radial wave function at the muffin-tin sphere radius corresponding to the Fermi energy.

$D_l$  is the logarithmic derivative of the radial wave function at the sphere boundary.

$V(S)$  is the muffin-tin potential at the sphere boundary.

$S$  is the radius of the muffin-tin sphere.

The above quantities are taken from the band structure results. We have calculated  $\lambda$  separately for zinc, cadmium and selenide atoms and for the  $T_c$  calculation (Eq. (8)) the mean value of  $\lambda$  is used<sup>[34]</sup>.

The average of the phonon frequency square is

$$\langle \omega^2 \rangle = \frac{1}{2} \theta_D^2 \quad (6)$$

The variation of Debye temperature with pressure  $\theta_D(P)$  is given by<sup>[34]</sup>

$$\theta_D(P) = \frac{\sqrt{E_F}}{\sqrt{E_F^o}} \frac{a_o}{a} \theta_D^o \quad (7)$$

where  $\theta_D^o$ ,  $a_o$  and  $E_F^o$  are normal pressure quantities<sup>[35]</sup>.

Normal pressure Debye temperature of ZnSe and CdSe are 271K and 220K respectively.

The McMillan's formula<sup>[36]</sup> used for  $T_c$  calculation,

$$T_c = \frac{\theta_D}{1.45} \exp \left[ \frac{-1.04(1+\lambda)}{\lambda - \mu^* (1+0.62\lambda)} \right] \quad (8)$$

gives the good estimate of the  $T_c$  value. Here  $\mu^*$  is the electron-electron interaction parameter which is estimated using the relation<sup>[37]</sup>,

$$\mu^* = \frac{0.26N(E_F)}{1+N(E_F)} \quad (9)$$



where  $N(E_F)$  is the density of levels per atom per eV at  $E_F$ .

With the results obtained from the self-consistent calculation, we have computed  $\theta_D$ ,  $\lambda$ ,  $\mu^*$  and  $T_c$  as a function of pressure using Eqs.(4 - 9). The onset of superconductivity occurs at  $(V/V_0)_s = 0.475$  for ZnSe and 0.525 for CdSe corresponding to the pressure 1.5 Mbar (Table.2). The calculated values at high pressure (NaCl) structure of ZnSe and CdSe are given in Tables. 3 and 4. As pressure increases our computed value of  $T_c$  increases and reaches a maximum value.

In ZnSe, the highest  $T_c$  obtained in NaCl structure is 6.627 K at 3 Mbar (Table. 3). In CdSe, the highest  $T_c$  obtained in NaCl structure is 4.030 K at 3 Mbar (Table. 4). The calculated  $T_c$  values depend more sensitively on changes in  $\lambda$  than  $\mu^*$ , indicating that these compounds are electron-phonon-mediated superconductors.

**Table 3.** Variation of  $T_c$  as a function of pressure for ZnSe in NaCl structure

Pressure P Mbar	$\lambda$	$\theta_D$ K	$\mu^*$	$T_c$ K
1.5	0.242	712	0.102	0.016
2.0	0.354	783	0.115	0.744
2.5	0.412	842	0.132	1.494
3.0	0.564	925	0.154	6.627

**Table 4.** Variation of  $T_c$  as a function of pressure for CdSe in NaCl structure

Pressure P Mbar	$\lambda$	$\theta_D$ K	$\mu^*$	$T_c$ K
1.5	0.273	656	0.118	0.025
2.0	0.328	721	0.124	0.220
2.5	0.483	796	0.135	3.646
3.0	0.536	858	0.162	4.030

**Table 5.**  $T_c$  - max values of ZnSe and CdSe in high pressure NaCl structure

Compound	$a_o$ a.u.	$B_o$ Mbar	$E_g$ eV	$T_c$ -max K
ZnSe	10.681	0.705	2.67	6.627
CdSe	11.441	0.572	1.70	4.030

Similar to alkali halides and group III-V compounds, group II-VI compounds come under the class of pressure induced superconductors [23, 34]. When pressure is increased  $T_c$  increases and reaches the maximum value in high pressure structure. The  $T_c$ -max values are given in Table.5 along with the other related parameters corresponding to them. From Table.5, it is noted that the  $T_c$ -max values are 6.627 K and 4.030 K for ZnSe and CdSe respectively. When lattice constant decreases  $T_c$ -max value increase in Table.5.

This reflects the fact that the structural and band gap configurations play an important role in the superconducting (high  $T_c$ -max) behaviour of these compounds under high pressure.

## 4. Conclusion

In the present investigation, the pressure dependent band structures and density of states of ZnSe and CdSe are computed and the results are used to study the metallization and superconductivity under high pressure for the first time theoretically. When the pressure is increased there is enhanced overlapping between the wave functions of the neighbouring atoms. As a result the widths of the valence and empty conduction bands increase. These changes lead to the narrowing and closing of band gaps in ZnSe and CdSe (metallization). On further increase of pressure, ZnSe and CdSe become superconductors, and these materials come under the class of electron-phonon-mediated high pressure superconductors. It is also confirmed that the metallization, structural phase transition and onset of superconductivity do not occur simultaneously in these compounds (Table.2).

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