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Theoretical Analysis of Elastic Properties of Zn*X* (*X* = Se and Te) under High Pressure

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ABSTRACT. We have evolved an effective inter ionic interaction potential to investigate the second order, third order elastic constants and Debye temperature for zinc blende (*B*3) structure in II-VI (ZnSe and ZnTe) semiconducting compound. The elastic properties were estimated by developing an interionic potential which includes the long range Coulomb, van der Waals (vdW) interaction and the short-range repulsive interaction upto second-neighbor ions within the Hafemeister and Flygare approach. We have also obtained thermodynamical parameters, such as, force constant, Gruneisen parameter, reststrahlen frequency and the compressibility. The variations of third order elastic constants with pressure follow a systematic trend identical to those exhibited by others compounds of *B*3 type structure family and the Born relative stability criteria is valid in Zn*X* (*X* = Se and Te) compounds.

Keywords: Elastic constants, Thermodynamical papameters, interionic interaction potential

I. INTRODUCTION

As semiconducting binary materials, Zn*X* (*X*= Se and Te) have grabbed the more attention in the last few decades. These compounds are used in several established commercial electronic and opto electronic devices, operating in blue to ultraviolet spectral regions such that visual displays, high-density optical memories, transparent conductors, solid-state laser devices, photo detectors, and solar cells. They crystallize in zinc blende (*B*3) structures [1-4]. at ambient pressure. The high pressure study of II–VI semiconductors has exhibited polymorphic structural transformation in these compounds. On one hand ZnSe is suited for the fabrication of blue light-emitting diodes in quantum well device. [5-7]. , On the other hand, ZnTe is used in many technological applications, for example photovoltaic devices, thin-film transistors, THz emitters, detectors and imaging systems [8]. .

The growth of the detect technology such as X-ray diffraction, thermoelectric, and Raman Spectra Measurement in high-pressure device has allowed us to determine the phase transition more exactly. However the two compounds are in the same family and have the same natural phase but their high pressure-induced phase transitions are not the same always. For example, ZnSe transform to rock-salt (*B*1) structure from natural phase (*B*3), whereas ZnTe shows a peculiar behavior under high pressure, transforming to the *B1* phase. Up to now, several experimental and theoretical results have been carried out on their phase transitions [9-14]. . By the phenomenological method, we have acquired the *B*3-*B*1 transition pressure at 15 GPa for ZnSe and 10 GPa for ZnTe earlier [15]. .

The anharmonic properties of crystalline solids give valuable information about inter atomic force along with thermal properties. Out of them the higher order elastic constants and the pressure derivatives of second order elastic are constants. As we are quite familiar with that cohesion in solids is vital than the most of the cohesion in these potentials is contributed by long range coulomb interaction, short range overlap repulsion explained by the Pauli exclusion principal [16,17]. . Born and Mayer have used overlap repulsion with a lattice sum to describe successfully the cohesion in most of the ionic solids [17]. . Earlier work of Fumi and Tosi [16]. , who properly included Van der Waals interaction along with dipole-dipole (*d-d*) and dipole-quadrupole (*d-q*) interactions to bring out the cohesion in several ionic solids. The Vander Waals coefficients are deduced from the SKV method [18]. . Here is becomes important to tell that the work of Singh [19]. who introduce the effects of three body interactions and follow Hafemeister and Flygare [20]. type overlap repulsion, extended up to second neighbour ions besides short-range interactions to discuss mechanical properties of several solids and alloys.

Hence the above approach successfully predicts thermodynamic properties in ZnX (X = Se and Te) compound. We have noticed that short range dipole-dipole (*d-d*) and dipole-quadrupole (*d-q*) interactions are the keystones for all of these approaches to to explain the cohesion of ionic solids. Present results are discussed in Section 2 and conclusion is in Section 3.

II. THEORY AND METHOD OF COMPUTATION

The understanding of thermo dynamical properties for ZnX (X = Se and Te) compound requires the formulation of an effective inter ionic potential. The effective inter ionic potential between pair of ions (i and j^{th}) is expressed as

$$U(r)=\sum_{ij}\frac{Z_m e^2}{r_{ij}}+\sum_{ij} b\beta_{ij}\exp\left(\frac{r_i+r_j-r_{ij}}{\rho}\right)+\sum_{ij} c_{ij}r_{ij}^{-6}+\sum_{ij} d_{ij}r_{ij}^{-8}. \tag{1}$$

Where, long-range Coulomb is represented by first term, second term correspond to Hafemeister and Flygare form of short-range repulsive energies [20]. and van der Waals multipole are represented by third and fourth terms, respectively. The Pauling coefficients β_{ij} are defined as: $\beta_{ij} = [1+(z_i/n_i)/(z_j/n_j)]$. with z_i (z_j) and n_i (n_j) as the valencey and number of outermost electrons in the anions (cations), respectively. The symbols: c_{ij} and d_{ij} are representing the dipole-dipole (*d-d*) and dipole-quadrupole (*d-q*) vander Waals coefficients. $Z_m e$ is the modified ionic charge due to Coulomb screening effects. and r_{ij} are the equilibrium distance between i^{th} and j^{th} ions. b (hardness) and ρ (range) are short-range parameters. Thus, the effective inter ionic potential contains only three free parameters (Z_m, b and ρ) which can be determined from the crystal properties [21]. .

A. Second and third order elastic constants

The study of the second-order elastic constants (SOEC) (C_{11}, C_{12} and C_{44}) , their pressure derivatives and third order elastic constants at 0 K is quite important for understanding the nature of the inter atomic forces in them. Since these elastic constants are functions of the first- and second-order derivatives of the short-range potentials, their calculations will provide a further check on the accuracy of short-range forces in these materials. We use the following second-order elastic constants (SOEC) for $B3$ phase:

$$C_{11}=\frac{e^2}{4a^4}\left[0.2477Z^2+\frac{1}{3}(A_1+2B_1)+\frac{1}{2}(A_2+B_2)\right], \tag{2}$$

$$C_{12}=\frac{e^2}{4a^4}\left[-2.6458Z^2+\frac{1}{3}(A_1-4B_1)+\frac{1}{4}(A_2-5B_2)\right], \tag{3}$$

$$C_{44}=\frac{e^2}{4a^4}\begin{bmatrix}-0.123Z^2+\frac{1}{3}(A_1+2B_1)+\frac{1}{4}(A_2+3B_2)\\ -\frac{1}{3}\left(-7.53912Z^2+A_1-B_1\right)\end{bmatrix}. \tag{4}$$

The expression for pressure derivatives of second order elastic constants follows

$$3\Omega\frac{dB_T}{dp}=-\left[20.1788Z^2-3(A_1+A_2)+4(B_1+B_2)+3(C_1+C_2)\right], \tag{5}$$

$$\begin{aligned}2\Omega\frac{d\sigma}{dp}=&-\left[-11.5756Z^2+2(A_1-2B_1)+\frac{2}{3}A_2-\frac{7}{2}B_2+\frac{1}{4}C_2\right],\\ &-\left\{\left[0.4952Z^2+\frac{1}{3}(A_1-4B_1+C_1)+\frac{1}{4}(2A_2-6B_2-C_2)\right]\right.\end{aligned} \tag{6}$$

$$\left.\begin{aligned}\Omega\frac{dC_{44}}{dp}=&+\nabla\left[-17.5913Z^2+A_1-B_2-\frac{2}{3}C_1\right]\\ &+\nabla^2\left[3.1416Z^2\frac{2}{3}(A_1-B_2)+\frac{C_1}{3}\right]\end{aligned}\right\} . \tag{7}$$

Furthermore, the expression for anharmonic third-order elastic constants, using the crystal potential and the method of homogeneous deformation leads to the following

$$C_{111} = \frac{e^2}{4a^4}\left[0.5184Z^2 + \frac{1}{9}(C_1 - 6B_1 - 3A_1) + \frac{1}{4}(C_2 - B_2 - 3A_2) - 2(B_1 + B_1)\right], \tag{8}$$

$$C_{112} = \frac{e^2}{4a^4}\left[0.3828Z^2 + \frac{1}{9}(C_1 + 3B_1 - 3A_1) + \frac{1}{8}(C_2 + 3B_2 - 3A_2)\right], \tag{9}$$

$$C_{123} = \frac{e^2}{4a^4}\left[6.1585Z^2 + \frac{1}{9}(C_1 + 3B_1 - 3A_1)\right], \tag{10}$$

$$C_{144} = \frac{e^2}{4a^4}\left[\begin{array}{l} 6.1585Z^2 + \frac{1}{9}(C_1 + 3B_1 - 3A_1) + \nabla\left[-3.3507Z^2 - \frac{2}{9}C_1\right] \\ + \nabla^2\left[-1.5637Z^2 + \frac{2}{3}(A_1 - B_1) + \frac{C_1}{9}\right] \end{array}\right], \tag{11}$$

$$C_{166} = \frac{e^2}{4a^4}\left[\begin{array}{l} -2.1392Z^2 + \frac{1}{9}(C_1 - 6B_1 - 3A_1) + \frac{1}{8}(C_2 - 5B_2 - 3A_2) - (B_1 - B_2) \\ + \nabla\left[-8.3768Z^2 + \frac{2}{3}(A_1 - A_2) - \frac{2}{9}C_1\right] + \nabla^2\left[2.3527Z^2 + \frac{C_1}{9}\right] \end{array}\right], \tag{12}$$

$$C_{456} = \frac{e^2}{4a^4}\left[\begin{array}{l} 4.897Z^2 + \frac{1}{9}(C_1 - 6B_1 - 3A_1) - B_2 + \nabla\left[-5.0261Z^2 - \frac{1}{9}C_1\right] \\ + \nabla^2\left[7.0580Z^2 + \frac{1}{3}C_1\right] + \nabla^3\left[-4.8008Z^2 + \frac{1}{3}(A_1 - B_1) - \frac{1}{9}C_1\right] \end{array}\right]. \tag{13}$$

Various symbols appear in the above expressions are associated with the crystal energy and have the following form

$$A_1 = A_{ij} = \frac{4a^3}{e^2}\left(\frac{d^2}{dr^2}V_{ij}(r)\right)_{r=a}, \tag{14}$$

$$A_2 = A_{ii} = A_{jj} = \frac{4a^3}{e^2}\left(\frac{d^2}{dr^2}V_{ii}(r) + \frac{d^2}{dr^2}V_{jj}(r)\right)_{r=a}, \tag{15}$$

$$B_1 = B_{ij} = \frac{4a^2}{e^2}\left(\frac{d}{dr}V_{ij}(r)\right)_{r=a}, \tag{16}$$

$$B_2 = B_{ii} = B_{jj} = \frac{4a^2}{e^2}\left(\frac{d}{dr}V_{ii}(r) + \frac{d}{dr}V_{jj}(r)\right)_{r=a}, \tag{17}$$

$$C_1 = C_{ij} = \frac{4a^4}{e^2}\left(\frac{d^3}{dr^3}V_{ij}(r)\right)_{r=a}, \tag{18}$$

$$C_2 = C_{ii} = C_{jj} = \frac{4a^4}{e^2}\left(\frac{d^3}{dr^3}V_{ii}(r) + \frac{d^3}{dr^3}V_{jj}(r)\right)_{r=a}, \tag{19}$$

$$\nabla=\left[\frac{-7.5391Z^{2}+\left(A_{1}-B_{1}\right)}{-3.141Z^{2}+\left(A_{1}+2B_{1}\right)}\right], \tag{20}$$

$$\Omega=-5.0440Z^{2}+\left(A_{1}+A_{2}\right)-2\left(B_{1}+B_{2}\right), \tag{21}$$

$$B_{T}=\frac{1}{3}\left(C_{11}+2C_{12}\right) \tag{22}$$

and

$$\sigma=\frac{1}{2}\left(C_{11}-C_{12}\right), \tag{23}$$

in terms of the short-range energy

$$V_{ij}(r)=\sum_{ij}b\beta_{ij}\exp\left(\frac{r_{i}+r_{j}-r_{ij}}{\rho}\right)-\sum_{ij}\frac{c_{ij}}{r_{ij}^{6}}-\sum_{ij}\frac{d_{ij}}{r_{ij}^{8}} \tag{24}$$

Here, b and ρ being the short-range parameters.

III. RESULT AND DISCUSSION

The effective interionic potential described in section (2) for the zinc blende ($B3$) phase contain three free parameters, which are , modified ionic charge, range and hardness parameters (Z_m, ρ and b). To estimate the free parameters, we first deduce the vdW coefficients from the Slater-Kirkwood variational method [18]. and are listed in table 1. We consider that the ZnX compounds to be partially ionic. For computation purposes we have deduced the values free papameters modified ionic charge (Z_m), range (ρ) and hardness (b) from the knowledge of equilibrium distance and the bulk modulus following the equlibrium conditions [21]. . The input data along with their relevant references and the model parameters for ZnX (X = Se and Te) compounds are given in table 2.

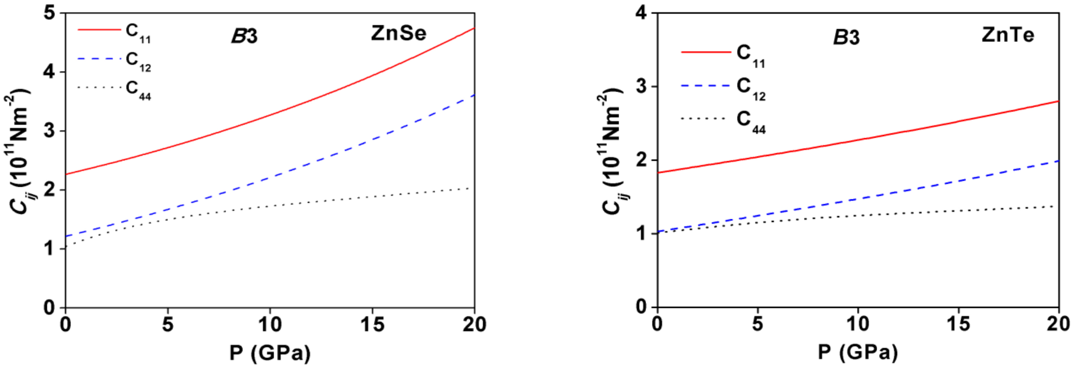
Table 1: The values of van der Waals coefficients c_{ij} (i,j = 1,2) [in units of 10^{-60} erg cm^6]. , d_{ij} (i,j = 1,2) [in units of 10^{-76} erg cm^8]. and overall van der Waals coefficients (C, D) for ZnX compounds.

Solids	vdW coefficients							
	c_{11}	c_{12}	c_{22}	C	d_{11}	d_{12}	d_{22}	D
ZnSe	38.04	112.82	533.96	709.24	12.07	115.26	702.23	586.33
ZnTe	38.04	149.11	1087.3	1078.1	12.07	197.0	1812.4	1100.3

Table 2: Crystal data and model parameters for ZnX (X = Se and Te) compounds.

	Material Parameters				Model Parameters		
	r_i(Å)	r_j (Å)	a (Å)	B_T (GPa)	Z_m^2	ρ (10^{-1} Å)	b(10^{12} erg)
ZnSe	0.74	1.73	5.667 [22].	62.67 [22].	3.24	3.9	2.148
ZnTe	0.74	1.83	6.089 [23].	52.80 [23].	3.35	4.1	2.55

While studying the high-pressure elastic behaviour of these compounds, we have computed the second-order elastic constants (SOEC) and their variations with pressure as shown in Fig. 1 (a, b). We have found that the value of C_{44} increase linearly with the increase of pressure from zero and does not tend to zero at the upto the pressure we studied, which is in accordance with the first order character of the transition and the values of C_{11} and C_{12} is also increase linearly with pressure. The variations of elastic constants with pressure follow a systematic trend identical to that observed in others compounds [21]. .



(a) (b)

Fig. 1 (a, b): Variation of second order elastic constant with pressure.

Further the stability of a cubic crystal is expressed in terms of elastic constants as follows [24]. :

$$B_T = (C_{11} + 2C_{12})/3 > 0, \tag{25}$$

$$C_{44} > 0, \tag{26}$$

and

$$C_S = (C_{11} - C_{12})/2 > 0. \tag{27}$$

Here, C_{ij} are the conventional elastic constants. Estimated values of bulk modulus B_T, shear moduli C_{44} and tetragonal moduli C_S are tabulated in table 3, well satisfy the above elastic stability criteria for Zn*X* (*X* = Se and Te) compounds. We analyze the anharmonic properties of Zn*X* (*X* = Se and Te) compounds by computing the third order elastic constants (TOECs) and the pressure derivatives of SOECs at zero pressure.The values of pressure derivatives of second order elastic constants as $d\sigma/dP, dB_T/dP$ and dC_{44}/dP for both two and three body interaction are listed in Table 3.

Table 3. The values of pressure derivatives of SOECs (dB_T/dP, dC_{44}/dP and dC_S/dP) and second order elastic constants (C_{11}, C_{12}, C_{44}) (in units of 10^{11} N m^{-2}).

Quantities	ZnSe	ZnTe
dB_T/dP	4.31	4.37
dC_S/dP	-0.25	-0.29
dC_{44}/dP	7.24	4.68
C_{11}	2.27	1.83
C_{12}	1.22	1.03
C_{44}	1.04	1.01
B_T	1.56	1.29
C_S	0.52	0.39

In continuation, the variations of third order elastic constants with pressure are shown in Fig. 2 (a, b). It can be seen that the variation of TOEC with pressure points to the fact that the values of C_{111}, C_{112}, C_{144}, $C_{166}$and C_{456} are negative, but the value of C_{123} is positive as obtained from the effective interionic potential at zero pressure.

Table 4. The values of third order elastic constants (C_{111}, C_{112}, C_{123}, C_{144}, $C_{166}$and C_{456}) (in units of 10^{11} N m^{-2}).

Quantities	**ZnSe**	**ZnTe**
C_{111}	-3.70	-3.19
C_{112}	-4.08	-3.48
C_{123}	1.80	-4.71
C_{144}	-3.15	-1.34
C_{166}	-7.68	-4.97
C_{456}	-3.63	-7.56

Furthermore, C_{166} and C_{144} increase, on the other hand, remaining third order elastic constants decreases with pressure and follows a systematic trend. Thus we can say that in ZnX, the developed interionic potential consistently explains the elastic behavior under high pressure.

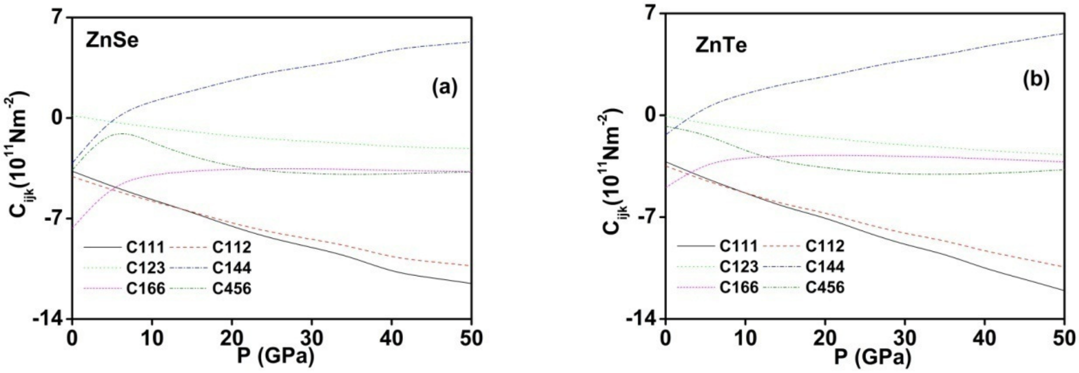


Fig. 2. Variation of third order elastic constant with pressure.

Apart from elastic constants, we have investigated various important physical properties like force constant (*f*), Gruneisen parameter (γ), Reststrahlen frequency (ν_0) and compressibility (β).The relevant expressions used in our calculations [27]. are given below. The molecular force in the absence of the Lorentz effective field is given by

$$f = \frac{1}{3}\left[\frac{d^2}{dr^2}U_{SR}(r) + \frac{2}{r_0}\frac{d}{dr}U_{SR}(r)\right]_{r=r_0} , \tag{28}$$

which consists of the short range overlap repulsion and the vdW interaction potentials between the unlike ions. The force constant in turn gives the Reststrahlen frequency as

$$\upsilon_0 = \frac{1}{2\pi}\left[\frac{f}{\mu}\right]^{1/2}, \tag{29}$$

with μ being the reduced mass.

In order to describe the anharmonic properties, we have calculated γ from the relation

$$\gamma = -\frac{r_0}{6}\left[\frac{U'''(r_0)}{U''(r_0)}\right], = \frac{3V\alpha_v}{\beta C_v} \tag{30}$$

$$\alpha_v = -\frac{C_v}{2r_0}\frac{U'''(r_0)}{[U''(r_0)]^2}, \tag{31}$$

Finally, the compressibility is

$$\beta = \frac{r_0^2}{9V}[U''(r_0)]. \tag{32}$$

The above thermodynamical parameters are listed in Table 5. We have used the effective interionic potential to successfully predicted the elastic and anharmonic properties of the test semiconducting compound under consideration. The dedused values of γ are consistent with the reported ones and this can be attributed to the proper incorporation of various interactions in the effective interionic potential.The present effective interionic potential consistently explain the high pressure, anharmonic behavior and associated thermodynamical variables of ZnX semiconducting compounds.

We have also estimated Debye temperature (θ_D) from the present approach. We define [27]. .

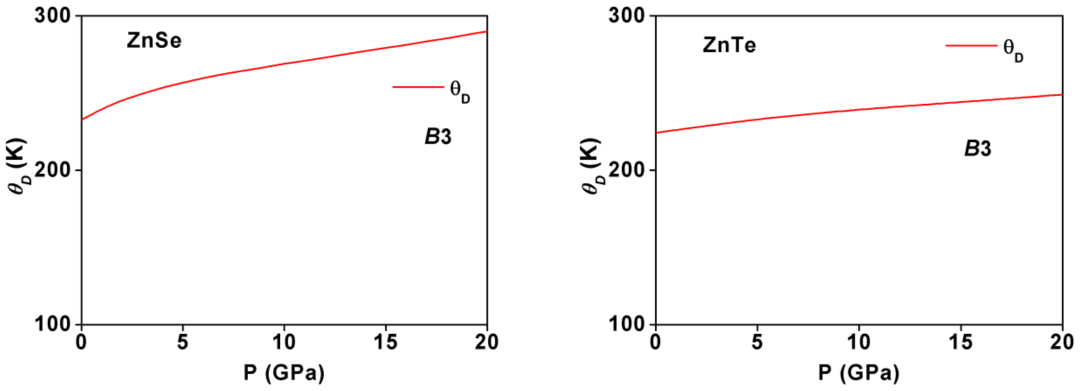
$$\theta_D^3 = \frac{3.15}{8\pi}\left(\frac{h}{k_B}\right)^3\left(\frac{r}{M}\right)^{\frac{3}{2}}(C_{11}-C_{12})^{\frac{1}{2}}(C_{11}+C_{12}+2C_{44})^{\frac{1}{2}}C_{44}^{\frac{1}{2}}, \tag{33}$$

Where M is the acoustic mass of the compound and h and k_B are the Planck and Boltzmann constant respectively. Fig. 3. show the variation of Debye temperature (θ_D) with pressure in $B3$ phase for ZnX (X = Se and Te) compounds. It is noticed from the figure that θ_D increases with increasing in pressure in $B3$ phase for ZnX (X = Se and Te) compounds and is attributed to softening of the lattice with pressure. The calculated values of the Debye temperature at zero pressure for ZnSe and ZnTe are 232.59 K and 224.11K respectively.

Table 5: Thermodynamical properties of ZnX (*X* = Se and Te) with zinc blende structure.

Properties	Formula	ZnSe	ZnTe
Force constant (f) (10^5dyne/cm)	28	3.70(4.59[a])	3.26(3.13[c])
Reststrahlen frequency (ν_0) (10^1	29	3.17(6.42[b])	2.98(5.20[b])
Gruneisen parameter (γ)	30	1.44(1.55[c])	1.48(1.58[d])
Compressibility (β) (10^{-11} Pa^{-1})	32	1.05	1.25

[a]Ref.[25]. , [b]Ref.[26]. , [c]Ref.[27]. , [d]Ref.[28].



(a) (b)

Fig. 3. Variation of Debye temperature (θ_D) as a function of pressure for ZnX (X = Se and Te) in B3 phase.

We do not claim the process to be rigorous, but a consistent agreement following effective interionic potential is obtained on Debye temperature as those revealed from experiments. Usually, the Debye temperature is also a function of temperature and varies from technique to technique and depends on the sample quality with a standard deviation of about 15 K.

IV. CONCLUSION

In this study, we have investigated the second-order elastic constants (SOEC), their pressure derivatives, third order elastic constants (TOECs), and Debye temperature (θ_D) of ZnX (X = Se and Te) compounds using developed model potential. We have checked the validity of Born criterion by computing second-order elastic constants that supports high pressure structural stability of ZnX (X = Se and Te) compounds. All the SOECs increase with increase in pressure and C_{44} does not tend to zero at the phase transition pressures. We should emphasize that our conclusions have been established only within the framework of interionic potential with overlap repulsion up to second nearest neighbor interactions. We also find that the variations of third order elastic constants with pressure points to the fact that the values of C_{111}, C_{112}, C_{144}, $C_{166}$and C_{456} are negative, but the value of C_{123} is positive as obtained from the effective interionic potential at zero pressure. The present study exhibits a quantitative description of the thermo-dynamical parameters of the selective semiconducting compound ZnX (X = Se and Te) and tests the suitability of the effective inter ionic potential.

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