CALCULATIONS OF THE STRUCTURAL, ELASTIC AND OPTICAL PROPERTIES OF ZnSe AT AMBIENT AND HIGH PRESSURE

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The structural, elastic and optical properties of ZnSe in the phases of (B3) zinc-blende and (B1) rock-salt are calculated by using the full-potential linear augmented plane wave (FP-LAPW) method based on the density functional theory (DFT) within the generalized gradient approximation (GGA). The calculated equilibrium lattice constant, bulk modulus, its pressure derivative and elastic stiffness coefficients are found in good agreement with the experimental and other theoretical data. The optical constants such as dielectric functions, refractive indices, reflectivity, absorption coefficient, optical conductivity, loss functions and extinction coefficient have been calculated for the photon energies up to 14 eV.

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1. Introduction

The zinc-selenide (ZnSe) semiconductor have received and still receiving considerable attentions due to its enormous technological importance. This environment friendly material is ideally suited for the fabrication of blue light emitting diodes (LED) and laser diodes [1-7]. It is also an important key material used for infrared windows, lenses, and prisms. ZnSe crystallizes either in the hexagonal wurtzite (B4) structure or the cubic zinc-blende structure (B3) or both type at ambient pressure. Under application of large external pressure, ZnSe transform into rock-salt (B1) structure. X-ray diffraction measurements show that ZnSe transforms from ZB to RS at 13.5 GPa in the upstroke, changing coordination from 4 to 6 [8-9]. By the Slater–Kirkwood variational method, Varshney et al obtained the ZB-RS transition pressure at about 18 GPa [10]. A. Stroppa et al have reported \textit{ab initio} pseudo potential calculations for the structural and electronic properties of ZnSe/GaAs(001) heterostructures with interface configurations accounting for charge neutrality prescriptions[11]. Structural properties, transition pressures and crystal stability have been discussed in several studies [12-17]. To the best of our knowledge the experimental studies of RS ZnSe is not available in the literature. Therefore, the main aim of our work is to investigate the structural, elastic and optical properties of ZnSe in zinc blende (B3) and rock-salt phase (B1). Determination of the elastic constants of a solid material is very important for the assessment of mechanical properties. It is well known that the mechanical properties of a material also changes when the phase transition takes place. The accurate measurement of these quantities is a very difficult task at high pressures of the experimental conditions. But with the \textit{ab initio} quantum mechanical methods we can calculate the elastic properties at ambient or elevated pressure conditions. This work presents a detailed study about the behavior of elastic, mechanical and optical properties of ZnSe in ZB and RS phases by using the first-principle calculations based on density functional theory (DFT) within generalized gradient approximation (GGA).

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This paper is organized as follows. Section II gives a description of the method as well as some details of the calculations. The calculated structural and mechanical properties of ZnSe are presented and discussed in the Section III and IV. The calculated optical properties have been presented in Section V. Finally, section VI contains the summary of obtained results and conclusion.

2. Computational Method

We have carried out our calculations with a self-consistent scheme by solving the Kohn-Sham equation using a FP-LAPW method within a framework of density functional theory (DFT) [18], as implemented in the WIEN2k code [19]. The generalized gradient approximation (GGA) [20-24] was used for the exchange-correlation potential. In the FP-LAPW method, the unit cell is partitioned into non-overlapping muffin-tin spheres around the atomic sites and in interstitial region. In these two types of regions, different basis sets are used. The wave function and potential are expended in spherical harmonic functions inside non-overlapping spheres and a plane wave basis set in the remaining space of the unit cell (interstitial region) is used. In the zinc-blende structure, the muffin-tin (MT) sphere radii of 2.32 a.u. and 2.06 a.u. were used for Zn and Se atoms respectively, while in the rock-salt structure 2.50 a.u. and 2.22 a.u. were used because the lattice constants of the two structures are different. The maximum l-value for the wave functions expansion inside spheres was confined to \( l_{\text{max}} = 10 \). The plane wave cut off of \( K_{\text{max}} = 8.0/R_{\text{MT}} \) (\( R_{\text{MT}} \) is the smallest muffin-tin radius) is chosen for the expansion of the wave functions in the interstitial region. The charge density was Fourier expanded up to \( G_{\text{max}} = 14 \). A mesh of 72 special k-points were taken in the irreducible wedge of the Brillouin zone for both B3 and B1 structure of ZnSe. In the present calculations, the core states are treated fully relativistically while the valence and semi core states are treated semi-relativistically (ignoring the spin-orbit coupling). The self-consistent is considered to be converged when the total energy of the system is stable within \( 10^{-5} \) eV. We have done our calculations by specifying the atomic positions, for zinc-blende structure, Zn atom is at the position of (0,0,0) and Se atom sitting at the position of \( (1/4,1/4,1/4) \) in primitive unit cell while for the case of rock-salt structure, Zn atom is at the position of (0,0,0) and Se atom is at the position of \( (1/2,1/2,1/2) \) in the primitive unit cell.

3. Structural properties

The volume optimization was performed using the lattice constant by taking the experimental value for both ZB and RS phases of ZnSe. The total energy as a function of the volume were used for the determination of theoretical lattice constant and bulk modulus. With this procedure, equilibrium lattice constant, bulk modulus and its pressure derivative are calculated by fitting the total energy to the Murnaghan’s equation of state [25]. The figures 1 and 2 represents the volume optimization for the zinc-blende and rock-salt structures of ZnSe.

![Fig. 1. Total energy versus unit cell volume of ZnSe in (B3) zinc-blende structure using GGA calculation](image-url)
Figure 2. Total energy versus unit cell volume of ZnSe in (B1) rock-salt structure using GGA calculation.

The table 1 gives the calculated equilibrium lattice constant $a_0$, bulk modulus $B_0$, its pressure derivative $B'_0$ of the bulk modulus with other theoretical and experimental works. It is clearly seen that the GGA over-estimate the lattice parameter. The calculated results have been found well consistent with general trends of these approximation. The calculated lattice constant is 1.5% larger than the experimental value for ZB and RS structure of ZnSe respectively. Furthermore, bulk modulus $B_0$ and pressure derivative $B'_0$ of the bulk modulus are found in good agreement with their experimental values.

**Table 1: Calculated equilibrium lattice constant ($a_0$), bulk modulus $B_0$, and the pressure derivative of bulk modulus ($B'_0$), the related experimental data, and the other theoretical works for ZB and RS phase of ZnSe at zero pressure**

<table>
<thead>
<tr>
<th>Phase</th>
<th>Method</th>
<th>$a_0$ (Å)</th>
<th>$B_0$ (GPa)</th>
<th>$B'_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zinc-blende (B3)</td>
<td>Present work</td>
<td>5.75</td>
<td>57.30</td>
<td>4.56</td>
</tr>
<tr>
<td></td>
<td>Other(Ref.26)</td>
<td>5.54</td>
<td>72.44</td>
<td>4.02</td>
</tr>
<tr>
<td></td>
<td>Expt.(Ref.27)</td>
<td>5.66</td>
<td>64.7</td>
<td></td>
</tr>
<tr>
<td>Rock-salt (B1)</td>
<td>Present work</td>
<td>5.38</td>
<td>75.59</td>
<td>3.60</td>
</tr>
<tr>
<td></td>
<td>Other(Ref.26)</td>
<td>5.17</td>
<td>90.72</td>
<td>4.92</td>
</tr>
<tr>
<td></td>
<td>Expt. (Ref.28)</td>
<td>5.29</td>
<td>104</td>
<td>-</td>
</tr>
</tbody>
</table>

In these calculation, the computed lattice parameters have been utilized in order to observe the success and consistency of the present model on the other physical properties of the ZnSe material.

4. Elastic properties

The elastic constants of solids provide a link between the mechanical and dynamical behaviours of a crystal, and they also give significant information concerning the nature of forces in solids. The deformation of material under any small stresses can be characterized by elastic constants. The effect of strain on the electronic properties is also important for accessing some knowledge of the mechanical properties of the materials. The cubic crystals have three independent elastic constants, namely $C_{11}$, $C_{12}$ and $C_{44}$. Therefore, in order to calculate these three constants we need only a set of three equations. Therefore, only three types of strain must be applied to the crystal structure. Thus, a set of three equations is required to determine the
constants. The first equation envolves for calculating the bulk modulus $B$ of the crystals. For a cubic crystal, the bulk modulus can be defined as

$$ B = \frac{(C_{11} - 2C_{12})}{3} $$  \hspace{1cm} (1)$$

A second one is associated with the relationship between $C_{11}$ and $C_{12}$ and can be obtained by applying a volume conserving tetragonal strain to calculate the shear elastic constant, $C_s = \frac{(C_{11} - C_{12})}{2}$. The strain tensor is given as

$$ \varepsilon = \begin{pmatrix} \delta & 0 & 0 \\ 0 & -\delta & 0 \\ 0 & 0 & \delta^2/(1-\delta^2) \end{pmatrix} $$  \hspace{1cm} (2)$$

Here, $\delta$ is the deformation parameter., the total energy of the system under the tetragonal shear strain is given by

$$ E(\delta) = E_0 + 2C_s V_0 \delta^2 + O(\delta^4). $$  \hspace{1cm} (3)$$

Where $E_0$ is the energy of unstrained state

- $C_s$ is the cubic shear constant
- $V_0$ is the zero strain volume.

And the last equation is associated with $C_{44}$. A parabolic fit to the strain energy vs. strain $\delta^2$ yields the result of shear elastic constant. To determine the pure shear elastic constant, $C_{44}$ we use volume conserving tetragonal strain tensor which is given by the relation

$$ \varepsilon = \begin{pmatrix} 0 & \delta/2 & 0 \\ \delta/2 & 0 & 0 \\ 0 & 0 & \delta^2/(4-\delta^2) \end{pmatrix} $$  \hspace{1cm} (4)$$

which yields the total energy as following

$$ E(\delta) = E_0 + \frac{1}{2} C_{44} V_0 \delta^2 + O(\delta^4). $$  \hspace{1cm} (5)$$

Kleinmann parameter is a significant parameter describing the relative position of the cation and anion sublattices using the following relation [30]

$$ \xi = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}}. $$  \hspace{1cm} (6)$$

Furthermore, there are also two approximation methods, which can be used to calculate the polycrystalline modulus, namely the Voigt method [33] and the Reuss method [28]. The subscripts V denotes the Voigt bound and R denotes the Reuss bound. Here, $G_R$ is Reuss modulus given as

$$ G_R = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3(C_{11} - C_{12})} $$  \hspace{1cm} (7)$$

and $G_V$ the Voigt modulus defined as
\[ G_v = \frac{1}{5}(3C_{44} + C_{11} - C_{12}). \]  

(8)

However, the shear modulus or modulus of rigidity \( G \) describes an object's tendency about the deformation of shape at constant volume, when acted upon by opposing forces. Hence shear modulus \( G \) can be given by the following expression

\[ G = \frac{G_v + G_R}{2}. \]

The anisotropy constant is given in the following relationship

\[ A = \frac{2C_{44} + C_{12} - C_{11}}{C_{11}}. \]  

(9)

As the anisotropy constant approaches to unity, the crystal goes to isotropic phase, and the gap between the bounds vanishes. Young's modulus, which is also known as the tensile modulus or elastic modulus. It is a measure of the stiffness of an elastic material and is a quantity used to characterize materials. In anisotropic materials, Young's modulus can have different values depending on the direction of the applied force with respect to the material's structure. If the material is stretched rather than compressed, it usually tends to contract in the directions transverse to the direction of stretching of the material. The Poisson ratio will be the ratio of relative contraction to relative stretching. In some rare cases, a material will actually shrink in the transverse direction when compressed (or expand when stretched) which will yield a negative value of the Poisson ratio. Hence, Young's modulus \( E \) and Poisson ratio \( \gamma \) are related to the hardness for polycrystalline materials. These quantities are calculated by the following relation [29].

\[ E = \frac{9BG}{3B+G}. \]

(10)

And

\[ \gamma = \frac{1}{2} \left( \frac{3B-E}{3B} \right). \]

(11)

The Poisson's ratio of a stable, isotropic, linear elastic material cannot be less than -1.0 nor greater than 0.5 because the requirement that the Young's modulus, the shear modulus and bulk modulus have positive values. Some materials have Poisson's ratio values ranging between 0.0 and 0.5. A perfectly incompressible material deformed elastically on the application of small strains would have a Poisson's ratio of 0.5. The elastic constants \( C_{ij} \) (GPa), bulk modulus \( B \) (GPa), shear modulus \( G \), Young modulus \( E \), anisotropic parameter \( A \), Kleinmann parameter \( \xi \) and Poisson ratio \( \gamma \) with pressures (GPa) for ZnSe in the ZB and RS phase have been calculated and presented in the table 2.

### Table 2. The Calculated Elastic Constants \( C_{ij} \) (GPa), Bulk Modulus \( B \) (GPa), Reuss Modulus \( G_R \), Voigt Modulus \( G_V \), Shear Modulus \( G \), Anisotropic Parameter \( A \), Kleinmann Parameter \( \xi \), Young Modulus \( E \) and Poisson Ratio \( \gamma \) for ZnSe in the ZB and RS Phase

<table>
<thead>
<tr>
<th>Phase</th>
<th>Method</th>
<th>( C_{11} )</th>
<th>( C_{12} )</th>
<th>( C_{44} )</th>
<th>( B )</th>
<th>( G_R )</th>
<th>( G_V )</th>
<th>( G )</th>
<th>( A )</th>
<th>( \xi )</th>
<th>( E )</th>
<th>( \gamma )</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZB</td>
<td>This work</td>
<td>84.0</td>
<td>49.0</td>
<td>55.8</td>
<td>60.7</td>
<td>29.7</td>
<td>40.5</td>
<td>35.1</td>
<td>0.91</td>
<td>0.69</td>
<td>88.3</td>
<td>0.25</td>
</tr>
<tr>
<td></td>
<td>Other (Ref. 13)</td>
<td>96.2</td>
<td>59.9</td>
<td>52.7</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.63</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Expt. (Ref. 29)</td>
<td>88.8</td>
<td>52.7</td>
<td>41.4</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>RS</td>
<td>Present work</td>
<td>133.6</td>
<td>43.39</td>
<td>-120.9</td>
<td>73.4</td>
<td>256.1</td>
<td>54.2</td>
<td>155.3</td>
<td>-2.4</td>
<td>0.47</td>
<td>273.3</td>
<td>-0.12</td>
</tr>
<tr>
<td></td>
<td>Expt.</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
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</tr>
</tbody>
</table>
It is obviously observed that the bulk modulus of the B1 structure is obtained more than B3 structures. The three elastic constants can be obtained from the second-order derivative of the total energy of the crystal under three type of strains, the volume change, the volume conserved rhombohedral and tetragonal strains. The calculated bulk modulus from the elastic constants were found consistent with those obtained from Murnaghan equation for the two structure of ZnSe. The elastic constants must satisfy the conditions of $C_{11}-C_{12}>0$, $C_{44}>0$ and $C_{11}+2C_{12}>0$ for stable cubic phase. The above conditions are satisfied by ZB-ZnSe structure, proved it mechanical stable at ambient pressure. In the rock-salt structure, $C_{44}<0$, the restriction are fulfilled. It can be concluded that the zinc-blende (B3) structure is stable at ground state while the rock-salt (B1) structure is not stable at zero pressure. The anisotropy factor, Kleinmann parameter, and poisson ratio for B3 structure is more than those for B1 structure. While the shear modulus and young modulus for B3 structure are found lower than B1 structure. To the best of our knowledge, values of elastic constants of RS-ZnSe have not yet been measured experimentally and theoretically. Hence comparison is not possible. The calculated some other structural parameters such as Kleinman parameter, Shear modulus, Reuss modulus, Voigt modulus and Anisotropy factor, Young modulus and Poisson ratio are presented in this work would helpfull to guide the experimentalist and for other theoretical calculations.

5. Optical properties

In this theoretical method, the dielectric function and other optical properties can be calculated by using the momentum matrix elements. The momentum matrix elements in the dielectric function have been calculated on a grid of 3000 special k-points for both ZB and RS ZnSe. The imaginary part of the dielectric tensor can be computed from the electronic band structure of solid. The optical properties can be obtained from the complex dielectric function. It can be expressed as

$$\varepsilon_{\alpha\beta}(\omega) = \text{Re} \varepsilon_{\alpha\beta}(\omega) + i \text{Im} \varepsilon_{\alpha\beta}(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega).$$

The dielectric function, $\varepsilon_2(\omega)$, is strongly correlated to the joint density of states (DOS) and transition momentum matrix elements. The real and imaginary parts of dielectric functions can be used to calculate the other optical parameters such as refractive indices, optical conductivities, absorption coefficient and extinction coefficient. The following well-known relations have been used [32] for the calculation of optical properties:

$$\text{Im} \varepsilon_{\alpha\beta}(\omega) = \frac{4\pi e^2}{m^2 \omega^2} \sum_{C,V} \int_0^\infty dk \langle c_k | P^\alpha | v_k \rangle \langle v_k | P^\beta | c_k \rangle (\varepsilon_{c_k} - \varepsilon_{v_k} - \omega)$$

$$\text{Re} \varepsilon_{\alpha\beta}(\omega) = \frac{2}{\pi} \int_0^\infty \frac{\text{Im} \varepsilon_{\alpha\beta}(\omega)}{\omega^2 - \omega^2} d\omega,$$

Where $c_k$ and $v_k$ are the electron states in the conduction and valence bands, respectively, with the wave vector $k$.

The optical conductivity is given by the relation

$$\text{Re} \sigma_{\alpha\beta}(\omega) = \frac{\omega}{4\pi} \text{Im} \varepsilon_{\alpha\beta}(\omega).$$

The refractive index, $n(\omega)$, is given by

$$n(\omega) = \sqrt{\frac{\varepsilon_1(\omega) + \text{Re} \varepsilon_\omega(\omega)}{2}}$$

The extinction coefficient, $k(\omega)$, is given by
The linear optical properties of cubic ZnSe in B3 and B1 phase has been investigated by calculating the optical parameters, dielectric function $\varepsilon(\omega)$, refractive index $n(\omega)$ and optical conductivity $\sigma(\omega)$, absorption $I(\omega)$, reflectivity $R(\omega)$, extinction coefficient $k(\omega)$, and eloss function $L(\omega)$. The figure 3(a) and 3(b) show the imaginary, $\varepsilon_2(\omega)$, and real, $\varepsilon_1(\omega)$, parts of dielectric function calculated for ZnSe in ZB and RS phases.

The analysis of $\varepsilon_2(\omega)$ spectra shows that the threshold energy occurs at 0.013 eV for both phases. It is clear from the figure 3(a) that the main peaks are located at about 3.83 eV and 5.35 eV for B3 and B1 of ZnSe. Below the main peaks, there exist one more peaks located around 6.95 eV and 4.85 eV for ZB and RS phase of ZnSe. The calculated real part of dielectric tensor is given in the figure 3(b) shows that the first main and highest peak value 10.41 and 17.81 of $\varepsilon_1(\omega)$ exists at energy 3.29 eV and 2.16 eV for ZB and RS phases respectively. The calculated static dielectric constant $\varepsilon_1(0)$ without any contribution from lattice vibration corresponding to the low energy limit of $\varepsilon_1(\omega)$ in the fig. 3(b), are presented with available experimental and other reported results in the table 3. We should emphasize that wide band energy gap yields a smaller value of $\varepsilon_1(0)$. It can be seen from the figure 3(c) that the threshold value of the absorption spectrum $I(\omega)$, is 0.4 eV and 0.3 eV, and increasing continuously up to a maximum at 4 eV and 5 eV.
eV corresponding to the B3 and B1 phases of ZnSe, respectively. As in the figure 3(d), the optical conduction starts with energy of about 0.013 eV for both ZB and RS phase. We notice that on increasing photon energy, the optical conduction will rise and will reach to the upper level in the energy range of 5.40 eV in B3 phase and 3.87 eV in B1 phase of ZnSe. The gap of energy is the main cause of starting of the optical conduction. As the excited electron have no enough energy to pass the energy gap and move to the conduction band. From the fig. 4(a), a strong reflectivity was noticed and its maximum occurs at 13.56 and 4.06 eV originated from interband transitions for ZB and RS phases of ZnSe, respectively. The refractive index spectra is represented in the figure 4(b). This shows that the refractive index is significant only up to 3.36 of ZB and 2.95 eV for RS phases, beyond this energy value it drops sharply. The calculated static refractive index 2.68 for ZB phase and 3.44 for RS phase of ZnSe are listed in table 3. The Figure 4(c) represents the extinction coefficient $k(\omega)$. The local maxima of the extinction coefficient $k(\omega)$ correspond to the zero of $\varepsilon_1(\omega)$ (5.67 eV) and (3.98) for ZB and RS phase of ZnSe respectively.

![Fig. 4. Calculated optical constants (a) Reflectivity $R(\omega)$, (b) Refractive index $n(\omega)$, (c) Extinction coefficient $k(\omega)$, (d) Eloss function $L(\omega)$.](image)

The electron energy loss function $L(\omega)$, is a significant factor related to the energy loss of fast electron traversing in the material and usually maximum at the plasma energy [30]. Electron energy-loss spectroscopy involves measurement of the energy distribution of electrons that have interacted with a specimen and lost energy due to inelastic scattering. The energy required for the excitation of bulk plasmons depends on the electron density in the solid. The positions of the single electron excitation peaks are related to the joint density of states between the conduction
and valence bands. The interband transitions, which consist mostly of plasmon excitations, the scattering probability for volume losses is directly connected to the energy loss function. Here the electrons, which excite the atoms and thus these electrons of the outer shell is called valence interband transitions or valence Loss. The electron energy-loss spectrum can be calculated from the following relations

\[
\varepsilon_{\alpha\beta}(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)
\]

\[
\text{EEL Spectrum} = \text{Im} \left[ -1/\varepsilon_{\alpha\beta}(\omega) \right] = \frac{\varepsilon_2^2}{\varepsilon_1^2 + \varepsilon_2^2} \tag{17}
\]

In Figure 4(d), the most prominent peak in the energy loss spectrum is associated with the Plasmon peak and located at 12.80 eV and 11.95 eV for ZB and RS phase of ZnSe respectively and the corresponding frequency is called plasma frequency \((\omega_p)\) [31]. At higher energies, typically a few hundred eV, edges can be seen in the spectrum, indicating the onset of excitations from the various inner atomic shells to the conduction band.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Calculation</th>
<th>Static dielectric constant (\varepsilon_1(0))</th>
<th>Refractive index (n(0))</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZB</td>
<td>This work</td>
<td>7.19</td>
<td>2.68</td>
</tr>
<tr>
<td></td>
<td>Exp.[Ref.27]</td>
<td>6.30</td>
<td>-</td>
</tr>
<tr>
<td>RS</td>
<td>This work</td>
<td>11.84</td>
<td>3.44</td>
</tr>
</tbody>
</table>

To the best of our knowledge, we are not aware any data related to the optical dispersions of ZnSe in high pressure rock-salt(B1) phase. So comparison is not possible. But our present work could be helpful for the researcher to perform more experiments in this direction and other theoretical calculations.

6. Conclusions

The first principle calculations based on the density functional theory (DFT) within generalized gradient approximation (GGA) have been performed to investigate the equilibrium lattice constant, elastic properties and optical properties of ZnSe in ZB and RS phases. The calculated lattice parameters were found well in agreement with the already available experimental and theoretical values. For the elastic properties, we have achieved good agreement between the calculated elastic constants with other available results. The predicted values of elastic constants \((C_{11}, C_{12}, \text{ and } C_{44})\) and bulk modulus B in both phases ZB and RS obey generalized elastic stability criteria except for \(C_{44}\) in RS phase. Furthermore, we also have calculated the Kleinman parameter, Shear modulus, Reuss modulus, Voight modulus and Anisotropy factor, Young modulus and Poisson ratio. The calculation shows a static refractive index of 3.44 and 2.68 and dielectric constant of 7.19 and 11.84 for the stable ZB and RS phases of ZnSe respectively.

References