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# A*b initio* calculation of the Structural, Mechanical and Thermodynamic Properties of Beryllium Sulphide (BeS)

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**ABSTRACT:** An *ab initio* plane-wave Pseudopotential calculations using the density functional theory (DFT) implementing the generalised gradient approximation (GGA) to study the structural, elastic constants, phonon dispersion curves, density of state and thermal properties of BeS. Also we calculated the shear modulus, Young's modulus, Poisson's ratio, and the Zener's anisotropic factors. The calculated properties are agreement with previous experimental and theoretical results. The quasi-harmonic approximation is applied to determine the thermal properties, and these properties are in good agreement with available literatures. The major results of the properties determined were discussed.

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**Keywords:** Poisson's ratio, Plane-Wave Pseudopotential, Quasi-Harmonic Approximation, Lattice Parameter,

**INTRODUCTION** As shown by an earlier study (Camp and Doren 1996) the alkaline earth sulphide BeS has unique properties that are quite different from those of the other compounds BeX (X = O, Se, Te) in the series. Also, according to Yim et al, (1972), Zachariasen (1926)[a-b] and Staritzky (1956), the beryllium chalcogenides elements only BeS, BeSe and BeTe have the structure of the zinc-blende (ZB), which is a common feature to many well-known II – VI and III – V semiconductors. In the works of (Luo et al (1994); (1995), Weir et al (1986) and Vassiliou and Ahrens (1981)), it was observed recently that pressure induced structural phase transition in SrSe, calcium chalcogenides (CaS, CaSe, CaTe) and MgTe have left the beryllium chalcogenides (BeS, BeSe, BeTe) and mangnesium chalcogenides (MgS, MgSe, MgTe) the only unknown members in the entire IIA – VI series in regards to high pressure phase transition sequence. Srivastava et al (2004), in their work, did a study on the structural, electronic and dynamical properties of Be-Chalcogenide materials by using the plane wave pseudopotentials, density functional theory, and a linear response approach. The structural phase transition and ground state properties, and pressure dependence of the band gap of the series of compounds BeS, BeSe and BeTe have been calculated by employing the first principles tight binding linear muffin-tin orbital method within the local density approximation (LDA) Kalpana et al (1998). Also the results of these calculated bulk modulus the pressure volume relation and the lattice parameters, were found to be in good agreement with the recent experimental results. In recent times, the fast growing research areas includes investigation of thin layers and multilayers with different alloys containing beryllium. In the works of Paszkowicz et al (1998), they report that a partial replacement of Zn with Be improves the properties of the device because of dominant covalent bonding and high cohesive energy of BeSe. Such substitution allows to extend the domain of structural and band-gap engineering of II-VI semiconductors towards lower lattice parameters and higher energy gaps. In the past decade, the electronic and structural properties of solids from first principle calculations has become possible to compute with great accuracy. From these computations the lattice constants, crystal structures, phonon spectra, bulk and shear moduli and other static and dynamical properties can be obtained and it is also possible to predict the properties of solid, which were formally not experimentally accessible. As a function of temperature, Lee and Xavier (1995), calculated the constant volume specific heat, the entropy, the phonon contributions to internal energy and Helmholts free energy and the atomic temperature factors of α–quartz and stishovite, two allotropic forms of $SiO_2$ from *ab initio* phonon band structures. To determine the phonon density of state, dispersion relations, decomposition density of states and thermal

quantities, Laref and Laref (2012) in their work, used the density functional perturbations theory with quasi-harmonic approximation QHA methods. In our present paper, we used an *ab initio* and quasi-harmonic approximations to study the structural, mechanical and thermodynamic properties of BeS using the density functional theory as viewed from the xcrysden software presented in Fig. 1.

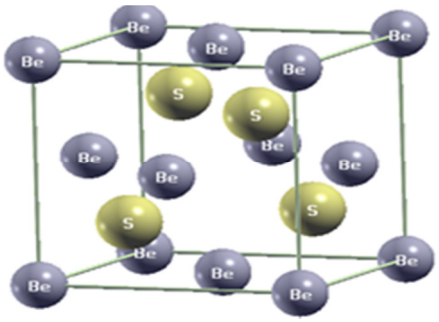


**Fig. 1.** Crystal structure of the BeS. The Be atoms form a face-centered-cubic (fcc) lattice.

## MATERIALS AND METHODS

*Total Energy Electronic Structure Calculation:* The first-principles calculations were performed using the QUANTUM ESPRESSO code (QE) as implemented in Baroni et al (2009), which has a basis set of a pane wave Pseudopotential PWPP method with the generalized gradient approximation GGA as reported in the works of Perdew et al (1996). In order to achieve convergence, a plane wave basis set with kinetic energy cut off of $612eV$, charge density cut off of $2449eV$ and convergence threshold of $1.0\times10^{-8}$ were applied and for the brillouin zone sampling, $8\times8\times8$ Monkhorst – Pack meshes for BeS was used. During the self-consistent calculation, the data set generated from the energy lattice parameter was fitted to the Birch third order Murnaghan equation of state and the equilibrium lattice constant, bulk modulus and pressure derivate of the bulk modulus were obtained.

*Elastic Properties:* We obtained the elastic constants after performing energy variation due to the applications of little strain to an optimized unit cell. According to Mehl (1993) and Wang and Ye (2003), the energy of a solid under stain is given as

$$\delta E = E_{tot} - E_0 = \tfrac{v}{2}\sum_{i=0}^{6}\sum_{j=0}^{6} c_{ij}e_i e_j \quad (1)$$

where $v$ is the volume of the equilibrium lattice cell, $\delta E$ is the energy increment from the strain with vector $e=(e_1,e_2,e_3,e_4,e_5,e_6)$ and $c$ is the matrix of the elastic constants. For cubic phases there are three independent elastic constants, $c_{11}$, $c_{12}$ and $c_{44}$. Its primitive vectors are defined as;

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 & \frac{\alpha}{2} & \frac{\alpha}{2} \\ \frac{\alpha}{2} & 0 & \frac{\alpha}{2} \\ \frac{\alpha}{2} & \frac{\alpha}{2} & 0 \end{pmatrix} \quad (2)$$

where $a$ is the lattice constant and the primitive vectors $a_1,a_2,a_3$ are transformed to the new vectors under strain by;

$$\begin{pmatrix} a'_1 \\ a'_2 \\ a'_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}(I+\varepsilon) \quad (3)$$

Where $\varepsilon$ is the strain tensor and $I$ is the identify matrix and it is related to the strain vector $e$ by;

$$\varepsilon = \begin{pmatrix} e_1 & \frac{e_6}{2} & \frac{e_5}{2} \\ \frac{e_6}{2} & e_2 & \frac{e_4}{2} \\ \frac{e_5}{2} & \frac{e_4}{2} & e_3 \end{pmatrix} \quad (4)$$

We apply the tri-axial shear strain $e=(0,0,0,\delta,\delta,\delta)$ to the crystal in the calculation of the elastic constants of the cubic phase. The $c_{44}$ can be calculated from;

$$\frac{\Delta E}{v} = \frac{3}{2}c_{44}\delta^2 \quad (5)$$

Also the shear modulus $G=\frac{1}{2}(c_{11}-c_{12})$ was obtained from the volume – conserving orthorhombic strain $\varepsilon=(\delta,\delta,(1+\delta)^{-2}-1,0,0,0)$ by using;

$$\frac{\Delta E}{v} = 6G\delta^2 \quad (6)$$

Hence $c_{11}$ and $c_{12}$ are given by;

$$c_{11} = \frac{3B+4G}{3} \quad (7)$$

$$c_{12} = \frac{3B-2G}{3} \quad (8)$$

Once the three independent elastic constants for cubic phases, $c_{11}$, $c_{12}$ and $c_{44}$, have been calculated parameters such as the Poisson's ratio $\mathcal{V}$, Young modulus $E$ and Zener anisotropy factor $A$ can be obtained from the following expressions:

$$\mathrm{V} = \frac{3B-2G}{2(3B+G)} \quad (9)$$

$$E = \frac{9GB}{3B+G} \quad (10)$$

$$A = \frac{2c_{44}}{c_{11}-c_{12}} \quad (11)$$

The relationship between the mechanical and dynamic behavior of the crystals can obtained from elastic constants, also vital information about the nature of the forces operating in the solids and the stability and

stiffness of the materials can be obtained. Hence, from the work of (Sinko and Smirnow 2002), for cubic crystals, the mechanical stability is measured by the following conditions: $c_{11} + 2c_{12} > 0$, $c_{11} - c_{12} > 0$, $c_{44} > 0$, and $c_{11} > 0$,(12)

*Thermodynamic Properties***:** The thermodynamic properties of BeS can be calculated by applying the quasi harmonic Debye model as reported in Chang et al., (2008). In the quasi-harmonic Debye model, the non-equilibrium Gibbs function $G*(V;P,T)$ is taken in the form of:

$$G*(V;P,T) = E(V) + PV + A_{vib}(\Theta(V);T) \quad (13)$$

where $E(V)$ is the total energy, $PV$ corresponds to the constant hydrostatic pressure condition $\Theta(V)$ is the Debye temperature. The adiabatic bulk modulus is given by;

$$B_s = B(V) = V\left\{\frac{d^2E(V)}{dV^2}\right\} \quad (14)$$

the isothermal bulk modulus $B_T$ and heat capacity $c_v$

$$B_T(P,T) = V\left(\frac{\partial^2 G*(V;T,P)}{\partial V^2}\right)_{P,T}$$

and $c_v = 3nK_B\left[4D(\Theta/T) - \frac{3\Theta/T}{e^{\Theta/T}-1}\right]$

## RESULTS AND DISCUSSION

*Structural Properties:* The equilibrium lattice constant $(a)$ has been determined by calculating the total energy at a range of lattice parameters around the experimental value within PWPP method with the generalized gradient approximation GGA, Perdew et al., (1996). We obtained the equilibrium lattice parameter $a$, the bulk modulus $B$ and the pressure derivative of the bulk modulus $B'$ by applying the fitting of the third order Birch-Mumaghan equation of state on the energy lattice parameters. We summarized our results, experimental values and other theoretical values as recorded in the works of Staritzky, (1956), Heciri et al, (2007), Narayana et al (1997), Laref and Laref, (2012), Guo et al., (2013), Okoye, (2004), Khenata et al., (2006), Benosman et al., (2001), and Gonzalez-Diaz et al., (1997) presented in Table 1(i). The optimized lattice parameter for the BeS compound in this work is consistent with the experimental values, although with slight discrepancy of about 0.0086%.

**Table 1.** Calculated lattice constant $a(\AA)$, bulk modulus $B(GPa)$ and its pressure-derivative $B'$ for BeS compared with other experimental and theoretical results. (i) (Structural Properties)

| Material (BeS) | $a(\AA)$ | $B(GPa)$ | $B'$ |
|---|---|---|---|
| Present work | 4.862 | 92.7 | 3.67 |
| Experimental'' | 4.862[a] | --- | --- |
| | 4.870[b] | --- | --- |
| Other theoretical | 4.878[c] | 93[c] | 3.524[c] |
| calculations | 4.83[d] | 93[d] | 3.33[d] |
| | 4.88[e] | 93.1[e] | 3.75[e] |
| | 4.88[f] | 92.23[f] | 3.07[f] |
| | 4.80[g] | 100.8[g] | 3.63[g] |
| | 4.819[h] | 1.13(Mbar)[h] | 3.99[h] |
| | 4.745[i] | 1.11(Mbar)[i] | --- |

a= Staritzky, (1956); b = Narayana et al, (1997), c= Heciri et al, (2007), d=Laref and Laref (2012), e=Guo et al, (2013), f=Okoye, (2004), g=Khenata et al, (2006), h = Benosman et al, (2001), i = Gonzalez-Diaz et al, (1997)

*Mechanical Properties***:** The investigation of the elastic constant requires knowledge of the shape of the energy curves as function of strain for unit cell. To determine the mechanical properties we have used the PWPP scheme following the method implemented in QE, by finite strain technique. We obtained values for the elastic constants: $c_{11}$, $c_{12}$, $c_{44}$, the Zener anisotropy $A$, the Poisson's ratio $\mathrm{V}$, Young modulus $E$ and the shear modulus $G$ by applying the equations (7-11) as stated in section 2.2. Our calculated values are in good agreement with previous theoretical results (See Table 1 and 2). The slight deviations are partly due to the calculation methods and fitting errors. And the stability conditions as in (Sinko and Smirnow, 2002) are all satisfied, which indicate that the compound BeS is mechanically stable at zero pressure and obeys the cubic stability conditions.

**Table 2.** Elastic constants: $c_{11}$, $c_{12}$, $c_{44}$, the Zener anisotropy $A$, the Poisson's ratio $\mathrm{V}$, Young modulus $E$ and the shear modulus $G$ for BeS compared with other experimental and theoretical results. (ii) (Elastic Properties)

| Material | $c_{11}(GPa)$ | $c_{12}(GPa)$ | $c_{44}(GPa)$ | $A$ | $\mathrm{V}$ | $E$ | $G$ |
|---|---|---|---|---|---|---|---|
| BeS | | | | | | | |
| Present work | 159.82 | 59.14 | 88.48 | 1.76 | 0.27 | 127.87 | 50.34 |
| Experimental | --- | --- | --- | --- | --- | --- | --- |
| Other theoretical | 146[c] | 67[c] | 103[c] | --- | --- | --- | --- |
| calculations | 157[d] | 61[d] | 97[d] | --- | 0.19[d] | 174[d] | 73[d] |
| '' | 158.2[e] | 61.1[e] | 92.7[e] | --- | --- | --- | --- |
| '' | 167[g] | 68[g] | 105[g] | --- | --- | --- | --- |
| '' | 1.87(Mbar)[h] | 0.75(Mbar)[h] | 0.82(Mbar)[h] | --- | --- | --- | --- |
| '' | 1.84(Mbar)[i] | 0.75(Mbar)[i] | 0.99(Mbar)[i] | --- | --- | --- | --- |

**Table 3.** Calculated phonon frequencies (in $cm^{-1}$) at the high – symmetry points $\Gamma$, $X$, $W$, and $L$ compared with other theoretical results.

| Material BeS | LO (Γ) | TO (Γ) | LO (X) | TO (X) | LA (X) | LO (L) | TO (L) | LA (L) | LA (L) |
|---|---|---|---|---|---|---|---|---|---|
| Present work | 524 | 524 | 647 | 493 | 370 | 240 | 601 | 531 | 371 | 173 |
| Other theoretical calculation | 655[a] | 566[a] | 611[a] | 548[a] | 364[a] | 163[a] | 656[a] | 513[a] | 367[a] | 229[a] |
| | 647[b] | 562[b] | 652[b] | 507[b] | 364[b] | 237[b] | 607[b] | 543[b] | 362[b] | 161[b] |
| | 652[c] | 562[c] | 654[c] | 505[c] | 357[c] | 226[c] | 607[c] | 545[c] | 361[c] | 158[c] |
| | 647[d] | 562[d] | 635[d] | 585[d] | 372[d] | 258[d] | 636[d] | 577[d] | 383[d] | 179[d] |

**Table 4.** Calculated values of $S$, $C_v$, $\Theta_D$, $\Delta E$ and $\Delta F$ at room temperature.

| Material, BeS | $S(J/mol.K)$ | $C_v(J/mol.K)$ | $\Theta_D(K)$ | $\Delta E(J)$ | $\Delta F(J)$ |
|---|---|---|---|---|---|
| Present work | 33.8 | 43.3 | 791 | 0.015 | 0.0087 |
| Other theoretical calc. | 30.7[d] | 36.3[d] | 782[d] | --- | --- |

*Phonon Dispersion Curves and Density of States*: We present the calculated phonon dispersion curves and the density of states curves in Fig 2 and Fig 3 respectively. In Table 3, our results presented are in good agreement when compared with available theoretical values. The longitudinal and transverse frequency modes of optical branch at $\Gamma$ point are in good agreement with the work of (Laref and Laref, 2012) but with slight deviation in the longitudinal optical. We noticed some features in the dispersion: Along the symmetry direction $\Gamma_{-L}$ the longitudinal optical $LO$ branch shows a sharp increasing amount of upward dispersion while the $TO$, a flat/horizontal dispersion it was also observed that the $LO$ and $TO$ branches did not cross. The calculated frequencies $TO$ and $LO$ at $\Gamma$ point coincide at $524cm^{-1}$ in this work, while the work of (Laref and Laref, 2012), there is a separation between $TO$ and $LO$ and they are $566cm^{-1}$ and $655cm^{-1}$ respectively, also from the work of Srivastava et al, (2004) the frequencies of $TO$ and $LO$ at $\Gamma$ point are $562cm^{-1}$ and $647cm^{-1}$. The disparity may be due to the type of k-point used in our calculation.

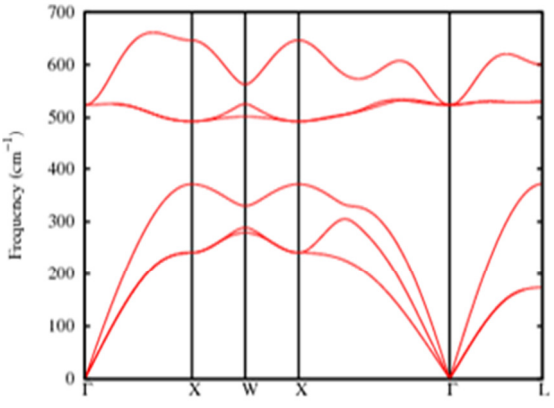


**Fig. 2** Calculated phonon dispersions curve for BeS.

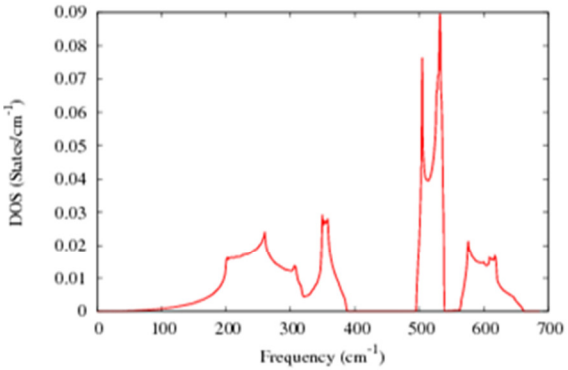


**Fig. 3**. Phonon density of states for BeS

*Thermodynamic Properties:* The thermodynamic properties of BeS have been investigated successfully. Figs 4 – 8 show the results of the Debye temperature $\Theta_D$, vibrational entropy $S$, specific heat at constant volume $C_v$, Free energy $\Delta F$, and the internal energy $\Delta E$ of the compound within a temperature range of 0 to $500K$. At high temperature $S$ and $C_v$ values increase sharply and eventually tends to a constant beyond $500K$. From the graph of Free energy $\Delta F$, with increasing temperature, the Free energy values reduce quickly and approaching zero beyond $500K$, while the internal energy increases slowly with temperature. At room temperature (300K), the calculated values of the $S$, $C_v$, $\Theta_D$, $\Delta E$ and $\Delta F$ are presented in Table 4. Also the Debye temperature $\Theta_D$ at minimum and $T \to 0$ are $684K$ and $970K$ is presented in Table 5.

**Table 5.** Debye temperature ( $\Theta_{D_{(\min)}}$ and $\Theta_{D_{(T\to 0)}}$ ) for BeS when compared with other theoretical results

| Material | $\Theta_{D_{(\min)}}(K)$ | $\Theta_{D_{(T\to 0)}}(K)$ |
|---|---|---|
| BeS | | |
| Present work (GGA) | 684 | 970 |
| Other theoretical calc. (LDA) | 608[d] | 748[d] |
| (LDT)[+] | 615[k] | 742[k] |

+ (k) Lattice dynamic theory, Wang and Ye, (2003)

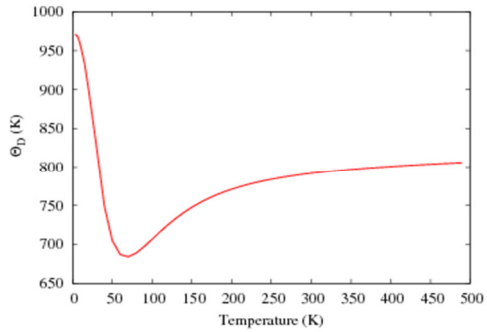


**Fig. 4**. The calculated Debye temperature within the range of (0-500K)

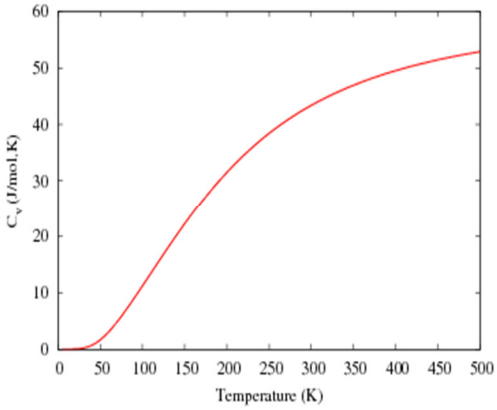


**Fig. 5.** Calculated specific heat at constant volume Cv (J/mo.K).

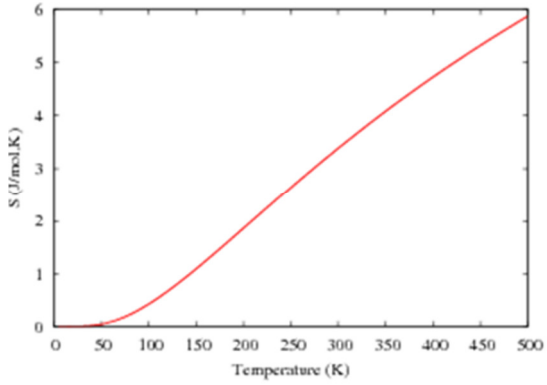


**Fig. 6**. The calculated vibrational entropy $S\ \ (J/mol.K)$ .

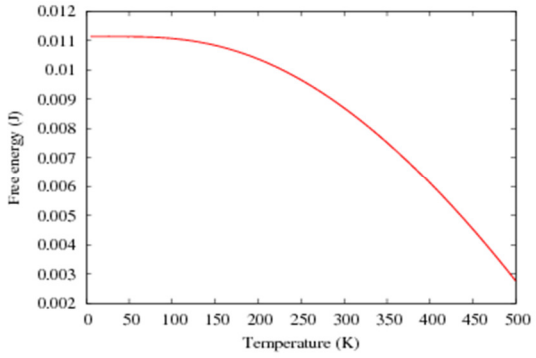


**Fig. 7**. The calculated Free energy ΔE (J) within temperature range (0 – 500) K

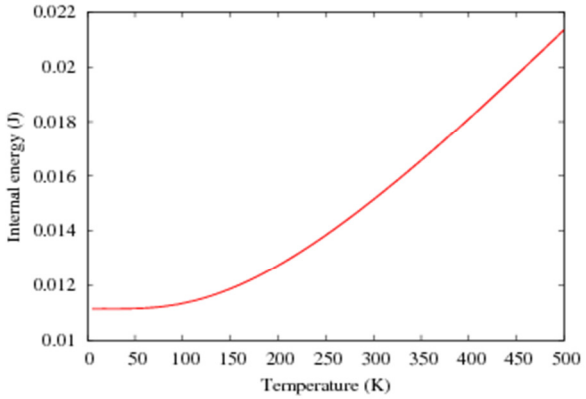


**Fig. 8**. The calculated Internal energy ΔF (J) within temperature range (0 – 500) K

**CONCLUSION** Our calculated value of B/G ratio of 1.8414 shows that BeS is ductile and capable of being shaped or bent and drawn out. Applying the cubic stability conditions, BeS is found to be mechanically stable. From the computed phonon dispersion curve and the thermodynamic properties it is observed that BeS is both stable lattice dynamically and thermodynamically respectively.

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