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Ab initio study of effect of pressure on structural and elastic properties of CaX, X = {O, S, Se}

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Abstract

We present density function theory study of effect of pressure on structural, elastic and electronics properties of compounds CaX (X=O, S and Se) within the generalized gradient approximation. The results presented for transition pressure, elastic parameters and band structures are in good agreement with the available literature. We also present the effect of pressure on these parameters. The generalized stability criteria show that CaSe is not stable above pressure of 29GPa and all the material CaX are not stable at B2 phase. The materials are brittle at equilibrium but this changes with pressure change. They are also generally anisotropic; CaO(B1) was found to be Isotropic at pressure of 12.5GPa. Finally, the band-gap of all the material around (Γ - X) decreased with pressure, all the material became indirect band-gap semiconductor at high pressure and CaSe undergoes a semiconductor-metal transition at pressure of 68 GPa.

Keywords: chalcogenide, brittleness, ductility, isotropic, brilliouin zone, band gap, malleability, pressure, GGA, elastic constant, lattice parameter.

Introduction

Chalcogenides based on alkali-earth metals have recently attracted more attention due to their flexibility and wide range of applications in areas such as; sensors, microelectronics, luminescence and in other devices that operate with high power input[1], [2]. These compounds crystallize in NaCl structure (B1) except few of them, like Beryllium MgTe [3]. Among these compound CaO, CaS and CaSe were found to undergo phase order transition from B1 phase to B2 phase [2][4]. These compounds are reported to be indirect band gap semiconductors [4-5]. A lot have been reported on these compounds [3]. Electronic band structure calculations for Calcium monochalcogenides, cohesive properties and behavior under pressure of CaS, CaSe and CaTe are reported by [33]. Theoretical study of CaO, CaS and CaSe via first-principle calculations [6], pressure induced structural, elastic and electronic properties of Calcium Chalcogenides via first principle calculation by [7], optical properties of alkali-earth metal Chalcogenides[8], structural and lattice dynamic of chalcogenides under pressure[1], [9], [10] and others [2], [5], [11]–[14] are noteworthy.

In this work, we report the study of the effect of hydraulic pressure on structural, elastic and electronic properties of Calcium Chalcogenides CaO, CaS and CaSe. This study is meant to complement other studies and add to already existing literature in this area.

Methodology

The study for effect of pressure on structural, elastic and electronic properties of Cubic Calcium Chalcogenides CaX (X = O, S and Se) which belong to space group 225 (Fm-3m) i.e. Chalcogenides in Rock salt structure (B1) and that of space group 221 (Pm-3m) i.e. Caesium Chloride structure (B2) were performed using ab initio method in the frame work of density function theory (DFT) as implemented in Quantum-Espresso [17, 18]. A generalized Gradient Approximation (GGA) was used with pw91 exchange-correlation function. A norm conserving pseudo-potentials were used with kinetic energy cut-off of 200Ry and a Brillouin zone sample of $8 \times 8 \times 8$. These settings where used for all the three Calcium (Ca) Chalcogenides (O, S and Se) throughout this paper except for the case of Density of the State (DOS) where Brillioun zone sample of $32 \times 32 \times 32$ were used.

The elastic constant calculation were performed using a package Thermo_pw which serves as an auxiliary plug-in to Quantum-Espresso in which crystal parameters can be utilized [20].

Result and Discussion

The investigation starts with determination of convergence of total energy with respect to kinetic energy cut-off as well as that of the Brillioun zone sampling (k-point) for CaX (X = O, S and Se). The result of these convergence test is presented in figure 1. The following is the convergence of kinetic energy cut-off and k-point mesh result for CaX, (X = O, S, Se).

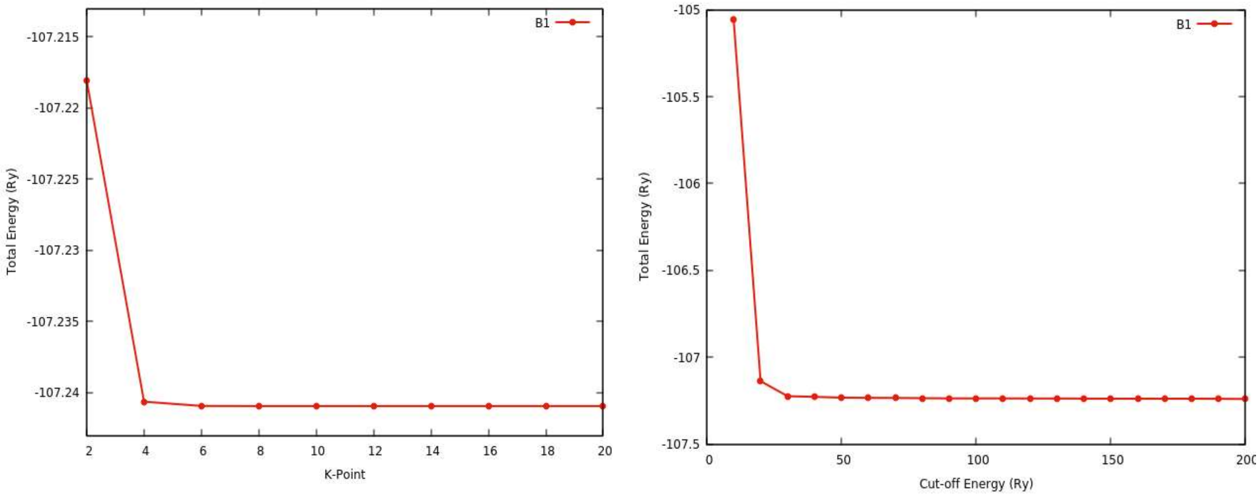

Figure 1: (a) Kinetic energy cut-off convergence with respect to total energy (b) Brillioun zone sampling forCaX (X = O, S, Se) with respect to total energy.

Materials are found to be in their natural state by minimizing their equilibrium energy to the barest minimum [4]. If material were found naturally to have many phases, the most stable phase is the one in which the material minimizes its energy more.

To find the most stable phase of these materials CaX, the total energy as function of their volume was plotted for the two phases Rocksalt (B1) and Caesium Chloride (B2) figure 2. It was found out that all the three compounds; CaO, CaS and CaSe preferred being in B1 structure (Natural form). This is in accordance with the work of[6], [10] among the others.

The effect of pressure on volume of the CaX (X=O, S and Se) was determined. The pressure applied (compression) to the Chalcogenides caused decrease of the lattice parameters, this corresponds to the decrease in volume of the compound. The percentage change in volume of Chalcogenides with respect to pressure is presented in figure 3.

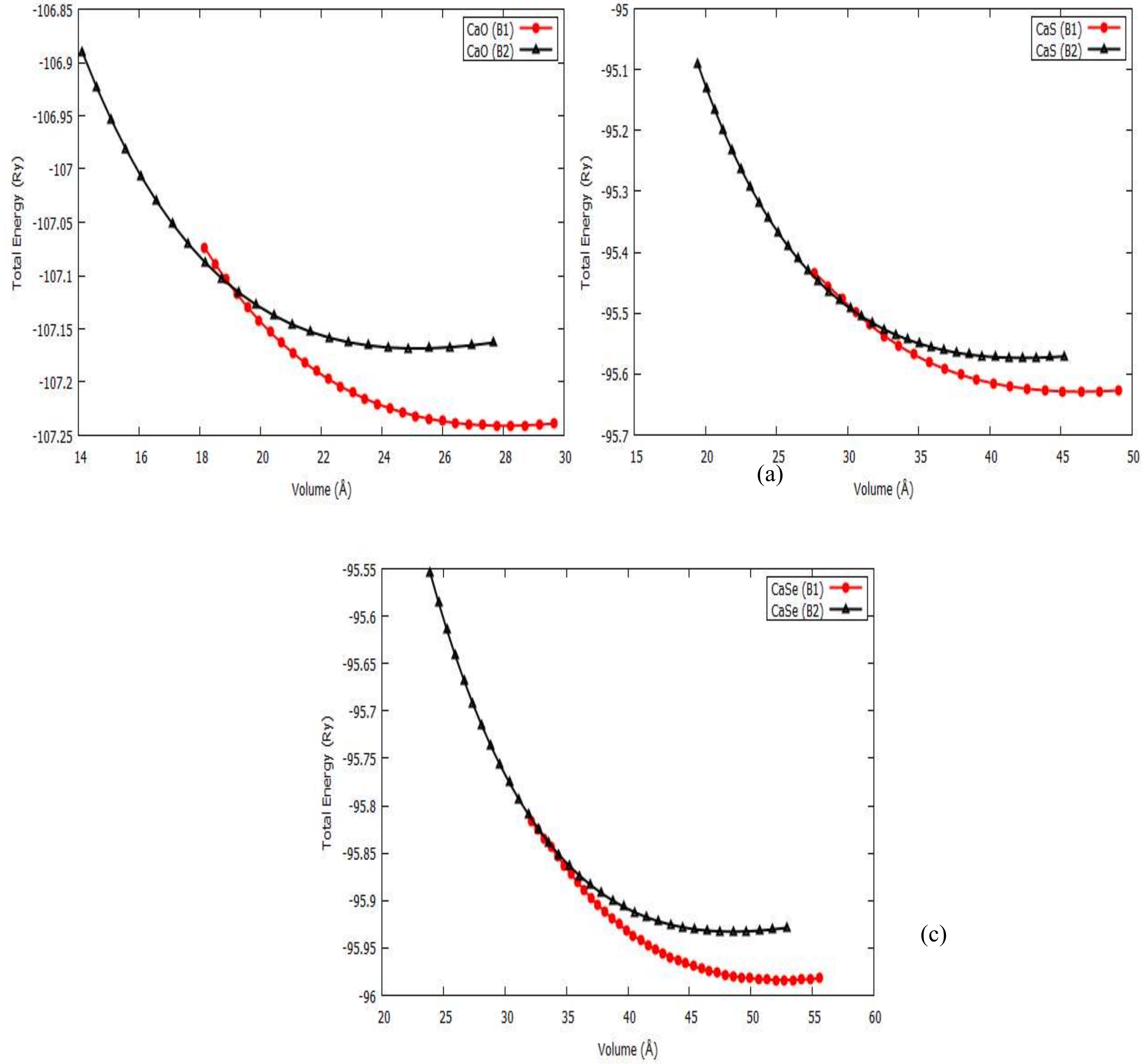

Figure 2: Energy as function of volume for the two phases of the CaX (B1 and B2) (a) CaO (b) CaS and (c) CaSe

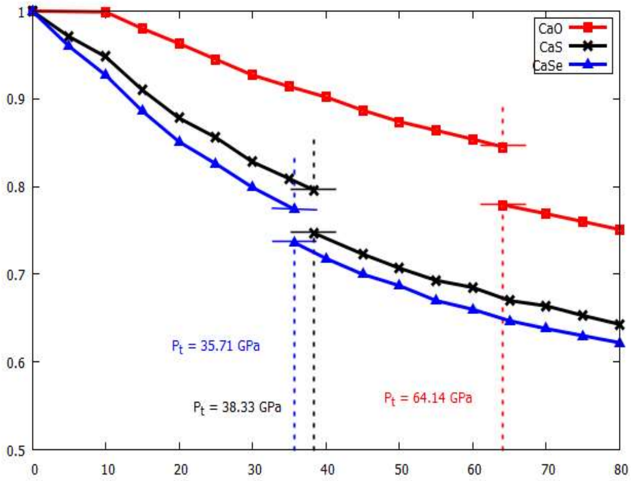

Figure 3: Effect of pressure on volume. (Pressure as a function of volume change)
For both B1 and B2 phases of the Compound CaX (X = O, S, Se and Te)

Phase Transition

Calcium Chalcogenides adopt Rock-salt structure (B1) with space group number 225 (Fm-3m) at equilibrium pressure, under compression the Chalcogenides undergo a first order transition to Caesium chloride Structure (B2) with space group number of 221 (Pm-3m). At zero temperature, Gibbs free energy is the same as enthalpy of a system. The Gibbs energy determines the structural stability for all possible phases of a given system. The difference in the enthalpy of the two phases B1 and B2 of these compounds CaX are plotted against pressure of the system as can be seen in figure 4, the transition pressures were hence determined.

Table 1 present the transition pressure, transition volume and ratio of transition volume of the two phases (B1) and (B2) to the equilibrium volume. The obtained parameters were in good agreement to both theoretical and experimental values. The transition pressures experimentally determine were accompanied with error values for CaO, CaS, and CaSe with transition pressures of$70 \pm 10, 37.1 \pm 2.9,$ and 33.9 ± 3.7 respectively

Table 1: Transition pressure $P_t(GPa)$ of the CaX, the transition volume $V_t(B_1)(\mathring{A}^3)$and $V_t(B_2)(\mathring{A}^3)$and the ratio of the transition volumes to equilibrium volumes ($V_t/V_0\ (B_1)$,$V_t/V_0\ (B_2)$ and $V_0\ (B_2)/V_0\ (B_1)$)

Parameters	CaO			CaS			CaSe		
	TW	Th.	Exp.	TW	Th.	Exp	TW	Th	Exp.
$P_t(GPa)$	64.14	32[38] 61[39] 75[40]	63[24] 60[25] 70[48]	38.33	35.39[31] 40[29] 49.8[60]	40[29] 37.1[40]	35.71	34.38[31] 40.65[31] 45[32]	38[29] 33.9[29]
$V_t(B_1)(\mathring{A}^3)$	19.25	20.7[42] 21.6[24] 20.9		30.18	33.640[5]	33.478[29]	33.07	37.55[5]	
$V_t(B_2)(\mathring{A}^3)$	16.06	18.542[5] 19.32[26] 19.3[37]		28.58	30.841[5]	30.048[29]	31.13	34.877[5]	
$V_t/V_0\ (B_1)$	0.69	0.73[5]	0.74[25]	0.65	0.721[5] 0.75[36] 0.71[34]	0.73[29]	0.63	0.705[5] 0.68[31] 0.75[35]	0.70[29]
$V_t/V_0\ (B_2)$	0.64	0.656[5]		0.67	0.661[5]		0.64	0.655[5]	
$V_0\ (B_2)/V_0\ (B_1)$	0.9			0.91	0.904[33]	0.9[51]	0.92	0.911[32]	0.91[51]

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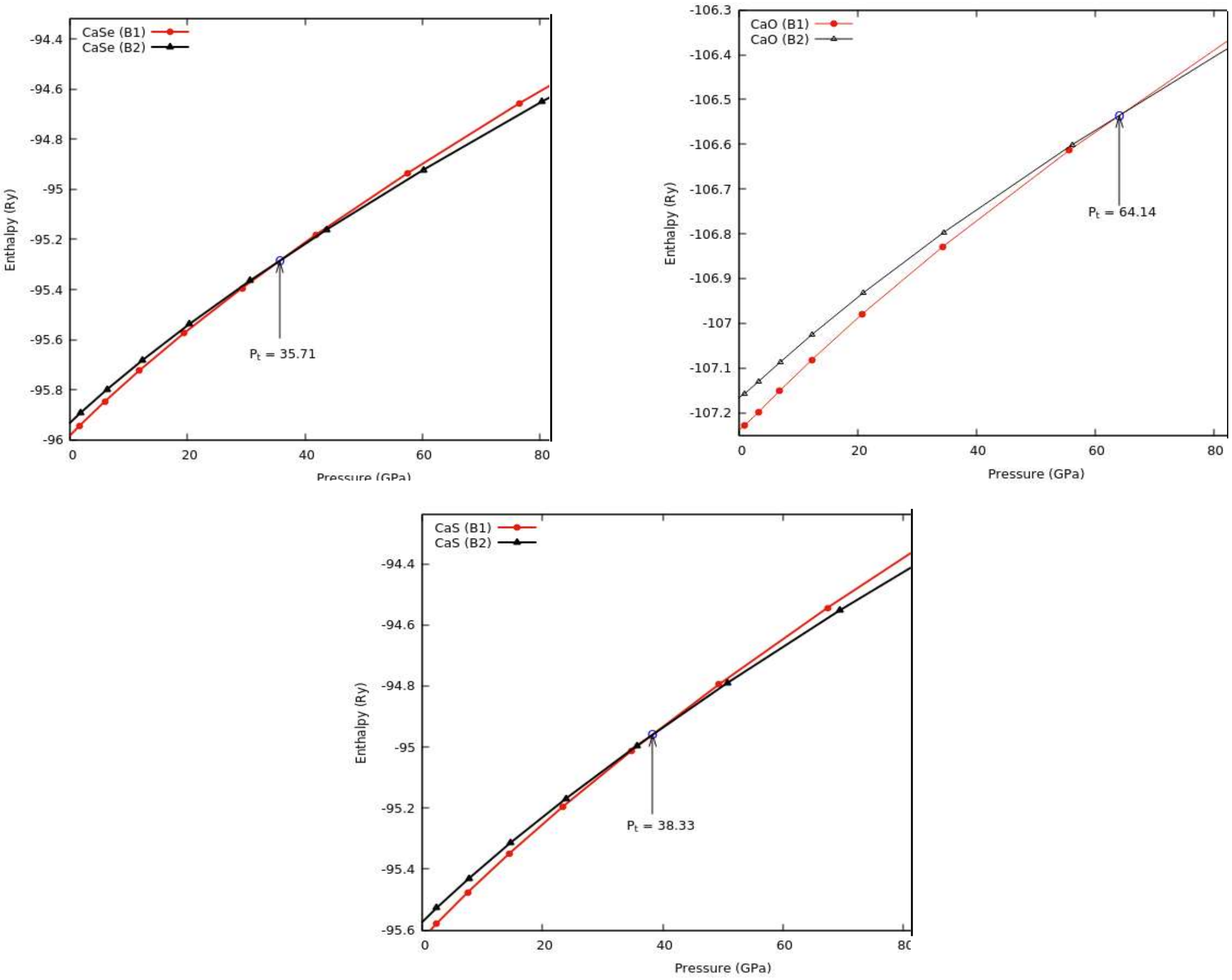


Figure 4: The Phase transition graph (Enthalpy as a function of pressure) From B1 phase of Chalcogenides to B2 phase (a) CaO (b) CaS and (c) CaSe

Equilibrium Parameters

At equilibrium; the lattice parameters, bulk modulus and its derivatives for these compounds CaX (X = O, S and Se) were determined and presented in table 2.

Table 2: Equilibrium parameters, the lattice constant$a_0(\AA)$, bulk modulus$B(GPa)$derivative of bulk modulus$B'$and elastic parameters$C_{11}C_{12}$andC_{44}

		CaO			CaS			CaSe		
Parameters		TW	Theor.	Exp.	TW	Theor.	Exp.	TW	Theor.	Exp.
			4.838[25]			5.717[31]			6.087[33]	
	B1	4.808	4.87[27]	4.811[24]	5.704	5.66[35]	5.69[32]	5.952	5.79[33]	5.916[53]
$a_0(\AA)$			4.65[26]			5.408[34]			5.71[34]	
			2.90[26]			3.494[31]			3.653[31]	
	B2	2.926	2.93[39]	2.907[25]	3.487	3.44[35]	3.460[30]	3.648	3.61[29]	3.611[53]
			2.85[37]			3.409[32]			3.559[32]	
			117[25]	111[25]		57.0[33]	64[30]		47.38[42]	
	B1	105.544	109[37[	115[24]	57.044	64[29]	56.3[31]	47.728	66[35]	51[53]
$B(GPa)$		114.701	129[35]		57.9646	67.4[43]		48.615	88.92[34]	
			113[39]			60.67[31]			51.41[33]	
	B2	107.752	119[46]	130[24]	61.038	65[35]	64[30]	50.880	58.65[48]	51[53]
		119.355	129[25]		69.168	77.42[43]		51.982	66.35[43]	
			4.08[38]	4.10[24]		3.8[31]	4.2[6]		3.34[42]	
	B1	4.283	4.41[26]	4.2[25]	4.135	4.10[29]	4.6[7]	4.265	4.4[43]	4.2[29]
B'			4.80[25]			4.6[30]			4.84[29]	
			4.3[37]			3.50[31]			3.6[59]	
	B2	4.285	4.4[38]	3.5[26]	4.022	4[35]	4.2[30]	4.134	4.2[53]	4.2[53]
			3.98[45]			5.4[43]			5.4[43]	
			239[26]	221[52]		108.23[48]			95.17[48]	
	B1	203.120	206[37]	223[49]	124.126	135[55]		105.149	115[55]	
$C_{11}(GPa)$			244.7[54]	226.2[53]		202.35[56]			155.25[56]	
	B2	360.840			184.626			153.0		
			108.23[26]	51.6[52]		32.01[48]			25.56[48]	
	B1	56.756	135[37]	50[49]	23.503	20[55]		19.017	18[55]	
$C_{12}(GPa)$			202.35[55]	23.9[53]		72.42[56]			55.75[56]	
	B2	-18.791			-0.756			-4.060		
			77.4[26]	80.30[52]		36.08[48]			27.11[48]	
	B1	76.259	66[37]	81.0[49]	33.791	38[55]		27.043	31[55]	
$C_{44}(GPa)$			99[54]	80.6[53]		67.45[56]			53.51[56]	
	B2	-13.128			-2.640			-2.550		

The obtained equilibrium parameters, lattice constant, bulk modulus, derivative of the bulk modulus and elastic constants are in agreement with the available experimental and theoretical result reported in the above table.

It is good to note that, the CsCl (B2) structures of the Chalcogenides CaX (X=O, S, Se) are not stable. This is because, the stability condition of these compounds at equilibrium which depends on elastic constant$C_{44}$is not satisfied in B2 phase (.i.e$C_{44} > 0$). Thus, the B2 phases of all the four Chalcogenides are not stable at equilibrium pressure (0GPa).

Stability

At zero pressure the Born stability criteria[15], [16] can be used to determine the stability of a crystal. [24] shows that, the Born criteria should be modified so as to capture the effect of pressure on the crystal, this criteria is modified to describe the changes in enthalpy not change in energy. Thus, the Born stability criteria and Generalized Stability criteria for a crystal under external pressure for a cubic crystal are given as:

The Usual Born Criteria are given by equation (1) – (3) below:

$$C_{11} + 2C_{12} > 0 \tag{1}$$

$$C_{11} - C_{12} > 0 \tag{2}$$

$$C_{44} > 0 \tag{3}$$

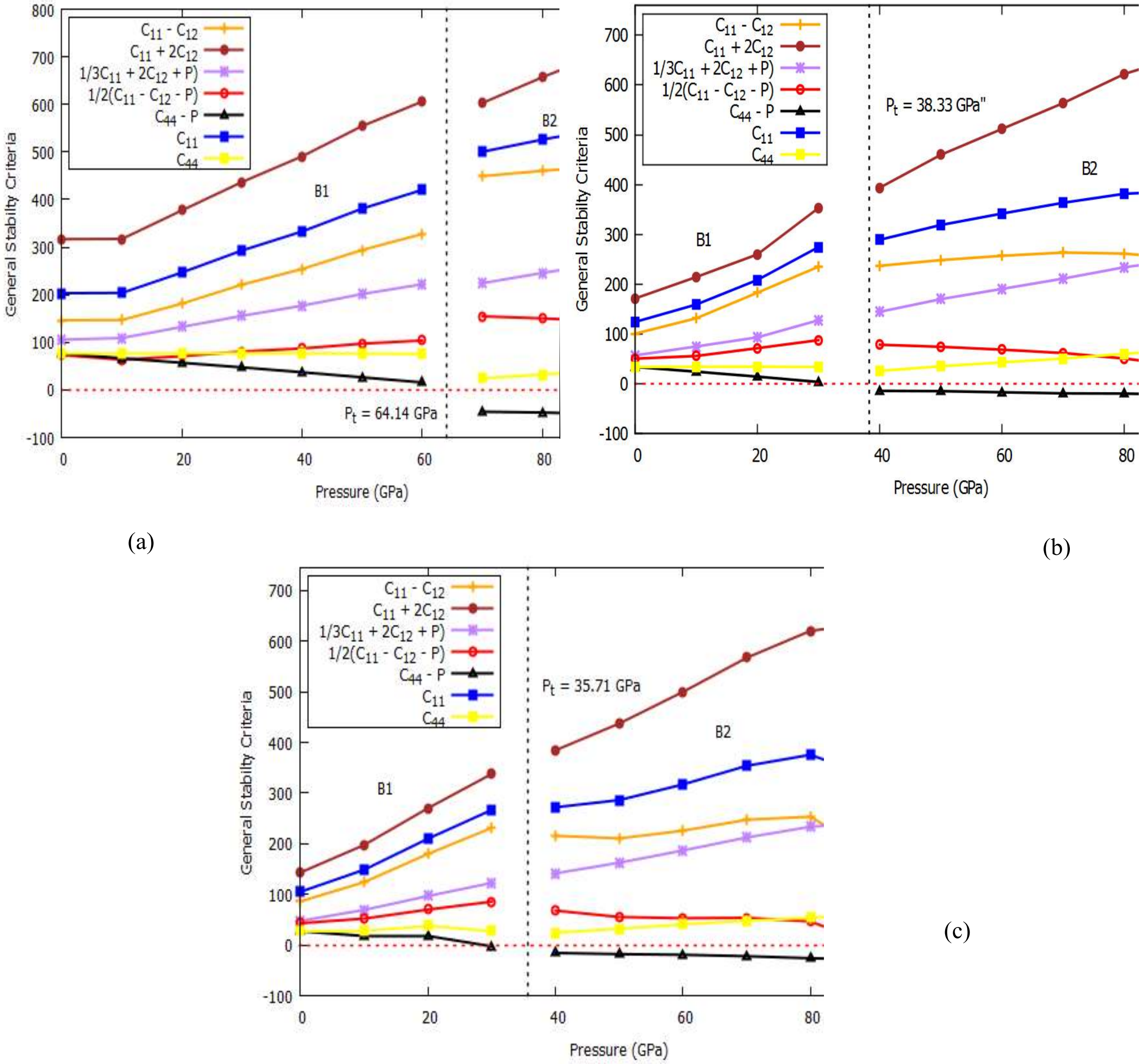
The generalized Stability Criteria are given s:

$$\frac{1}{3}(C_{11} + 2C_{12} + P) > 0 \tag{4}$$

$$\frac{1}{2}(C_{11} - C_{12} - P) > 0 \tag{5}$$

$$C_{44} - P > 0 \tag{6}$$

Born criteria, Generalized stability criteria and Crystal under external pressure are presented in figure 4. It can be seen that, if usual criteria will be considered by application of external pressure, all the three conditions equation (1) – (3) will be satisfied. But upon considering the generalized criteria highlighted by [24], equation (4) is satisfied for all the compounds CaX in the two phases. Equation (5) is satisfied for CaO and CaS in B1 and B2 phase while CaSe failed to satisfy the equation at pressure of 56GPa in B2 phase. Equation (6) is also satisfied for CaO and CaS in B1 phase, it failed at pressure of 29GPa for CaSe. The equation (6) failed in all the three compounds CaX in B2 phases. This shows that, the B2 phases of these materials are not stable. It also revealed that, even the stable B1 phase for the case of CaSe became unstable when external pressure is 29GPa, this is in agreement with the work of [7].



(a)

(b)

(c)

Figure 4: General stability condition for zero pressure (Born Stability Criteria) and for other (Wang, 1993) as function of pressure for the four Compounds CaX (X = O, S and Se) for both phases of the compounds (B1) and (B2). With (a) CaO, (b) CaS, and (c) CaSe

(c)

Mechanical Properties

Material moduli can be used to evaluate the mechanical properties of a material this include Bulk modulus ***B***, Young modulus ***E*** and Shear modulus ***G***. These properties reflect directly the material resistance to bulk, shear and elastic deformation[4]. Moreover, large modulus relate to high resistance to deformation. The material moduli can easily be determine from elastic constant C_{ij}.

Elastic Constant

Elastic constant were calculated initially for the equilibrium condition (0GPa) and re-calculated for the pressure difference between 0 and 80GPa. The effect of this pressure on elastic parameters were determined. The elastic constant determined (C_{ij}) were used to determine material moduli (B, E, and G) for the four Chalcogenides. The formulation as described somewhere by [23] are given in the following equations for a cubic crystal:

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \tag{7}$$

$$E = \frac{9BG}{3B + G} \tag{8}$$

$$G = \frac{1}{2}(G_a + G_b) \tag{9}$$

Where: $G_a = \frac{1}{5}(C_{11} - C_{12} + 3C_{44})\ is\ Voig\ shear;\ modulus$ and

$$G_b = \frac{5(C_{11} - C_{12})C_{44}}{\left(4C_{44} + 3(C_{11} - C_{12})\right)}\ is\ Reuss\ shear\ modulus$$

Figure 5 shows the calculated elastic constants and materials moduli for the three compounds under external pressure. In all the three Chalcogenides CaX, C_{11} varies greatly under pressure as compared to variation of C_{12} and C_{44} under influence of same external pressure. This is an indication that, all the Chalcogenides present a good resistance to change in their length, this is also observed and reported by[7]. The bulk modulus, young modulus and shear modulus vary under pressure for the two phases in the same trend for the case of CaO and CaS. For the CaSe the variation differs a little in the second phase B2 this can also be attributed to the fact that the materials are not very stable in the phase and for the second phase is almost similar. It is worth noting that, C_{44} is not very much affect by pressure change especially in B1 phase of the materials. These results are in good term with those reported by [7]. The modulus ratio B/G represent the Ductility/Brittleness of a material, it is a vital transition mechanism during phase change of materials. The ratio of modulus B/G can be used to describe the ductile/brittle properties of a material [4]. With B/G = 1.75 been critical value which distinguish between ductility and brittleness of a material [4]. When B/G of a material < 1.75, the material present brittle property and when B/G > 1.75 it is ductile. These properties increases as you move away from the critical value, that is, more brittle far less than 1.75 and more ductile for greater than 1.75. Figure 6(a) present the modulus ratio (B/G) and 6(b) the Poisson ration.

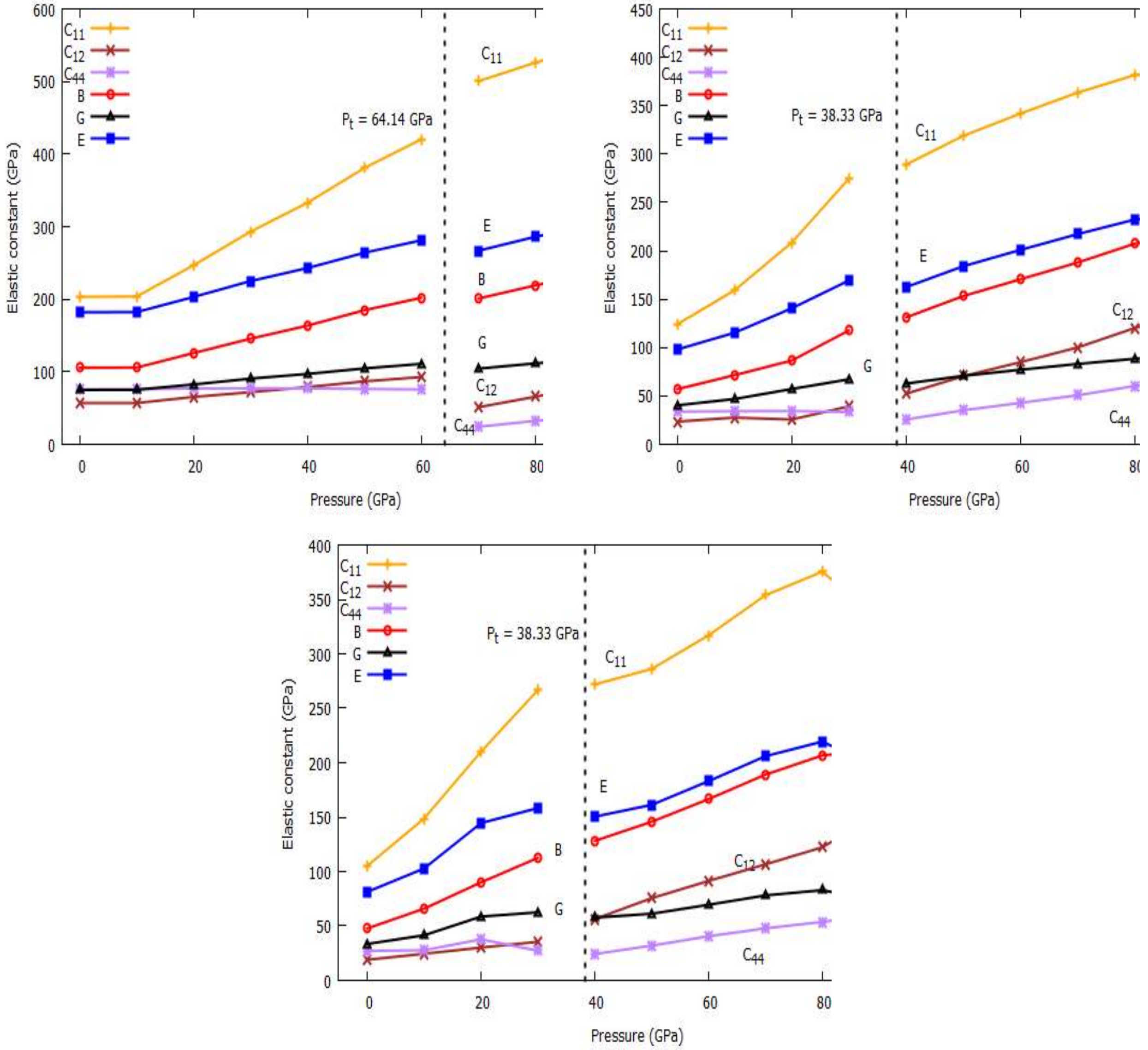


Figure 5: Elastic constant (C_{ij}), Bulk modulus (B), Shear modulus (G) and Young Modulus (E) as function of pressure for the four Chalcogenides CaX (X = O, S, Se and Te) for both phases of the compounds (B1) and (B2). With (a) CaO, (b) CaS and (c) CaSe

It can be seen that all the materials CaX are brittle at equilibrium, this properties changes with change in pressure in which CaO and CaS change from brittle to ductile at pressure of 47.45GPa and 29.98GPa respectively. It is good to mention that, the pressure at which these material became ductile decrease in the order CaO → CaS → CaSe. The Poisson ration is given by the following equations;

$$\sigma = \frac{C_{12}}{C_{12} - 2C_{44}} \tag{10}$$

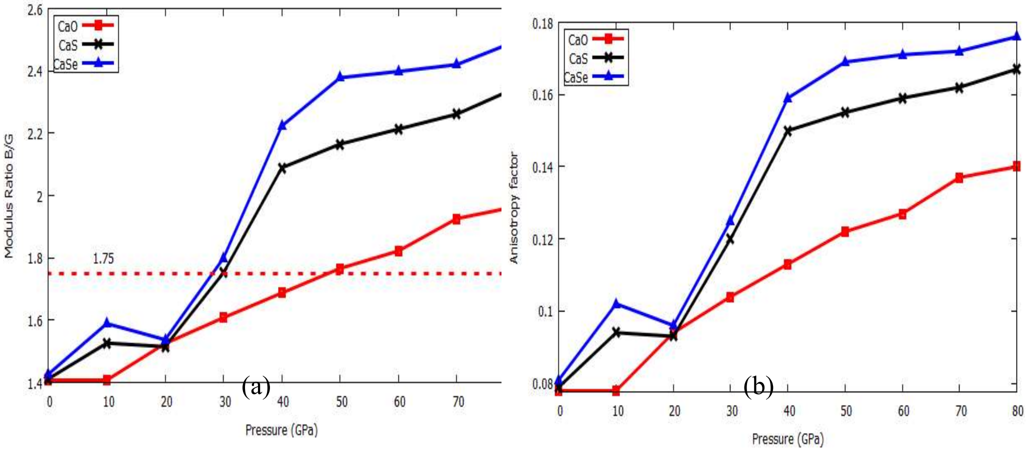


Figure: (a) Modulus Ratio B/G and (b) Poisson ration as function of Pressure for CaX (X = O, S and Se)

The calculated values of Poisson ratio as a function of pressure was presented in figure 6(b). This ratio is used to characterized the elastic properties of materials also. A material which is completely brittle the Poisson ratio is zero whereas for a ductile material is 0.5. When Poisson ration is small 0.1 – 0.25 the material can fracture easily whereas for range between 0.35 – 0.5 indicate the material will be hard to fracture [19]. This explain the reason why the two figures 6(a) and 6(b) are almost alike since they are describing similar properties.

Anisotropy Constant

Anisotropy constant A is used to describe elastic anisotropy of a material for a anisotropic materials. When this factor is unity ($A = 1$), the materials is said to be Isotropic, when this factor is not unity($A \neq 1$)the material is anisotropy [4][21][22]. The degree of anisotropy of a given material depends of the magnitude of the anisotropic factor A. figure 7 (a) – (c) show the anistropic factor A as function of pressure for the three compounds CaX. The degree of anisotropy of these materials

CaX (X = O, S and Se) decrease and increases with pressure for B1 and B2 phases of Chalcogenides respectively. For the case of CaO in B1 phase and CaS in B2 phase, at pressure of 12.5 GPa and 97GPa these materials exhibited Isotropic properties.

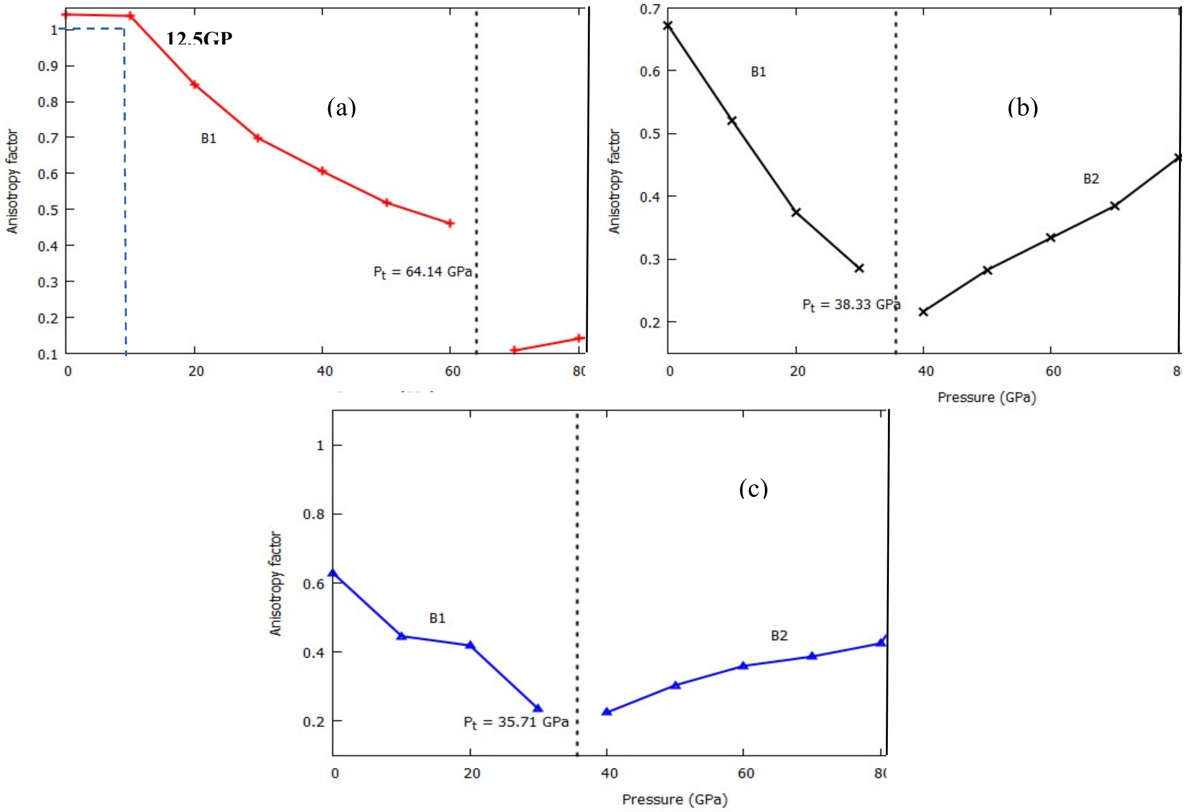


Figure 7: Anisotropy factor as a function of pressure for the four Chalcogenides CaX (X = O, S and Se) with (a) CaO, (b) CaS and (c) CaSe

Electronic Properties

The CaO, CaS and CaSe are indirect band-gap semiconductors with minimum conduction band and the maximum valance band at*Γ*and X point. The calculated band-gap decreases in the order CaO → CaS → CaSe with values at equilibrium of 3.69eV, 2.40eV and 2.06eV respectively, this is in agreement with the work reported by[7], [14].

Figure 8 (a) - (f) shows the equilibrium band structure with the corresponding density of the state (DOS) for Chalcogenides CaX (X = O, S and Se).

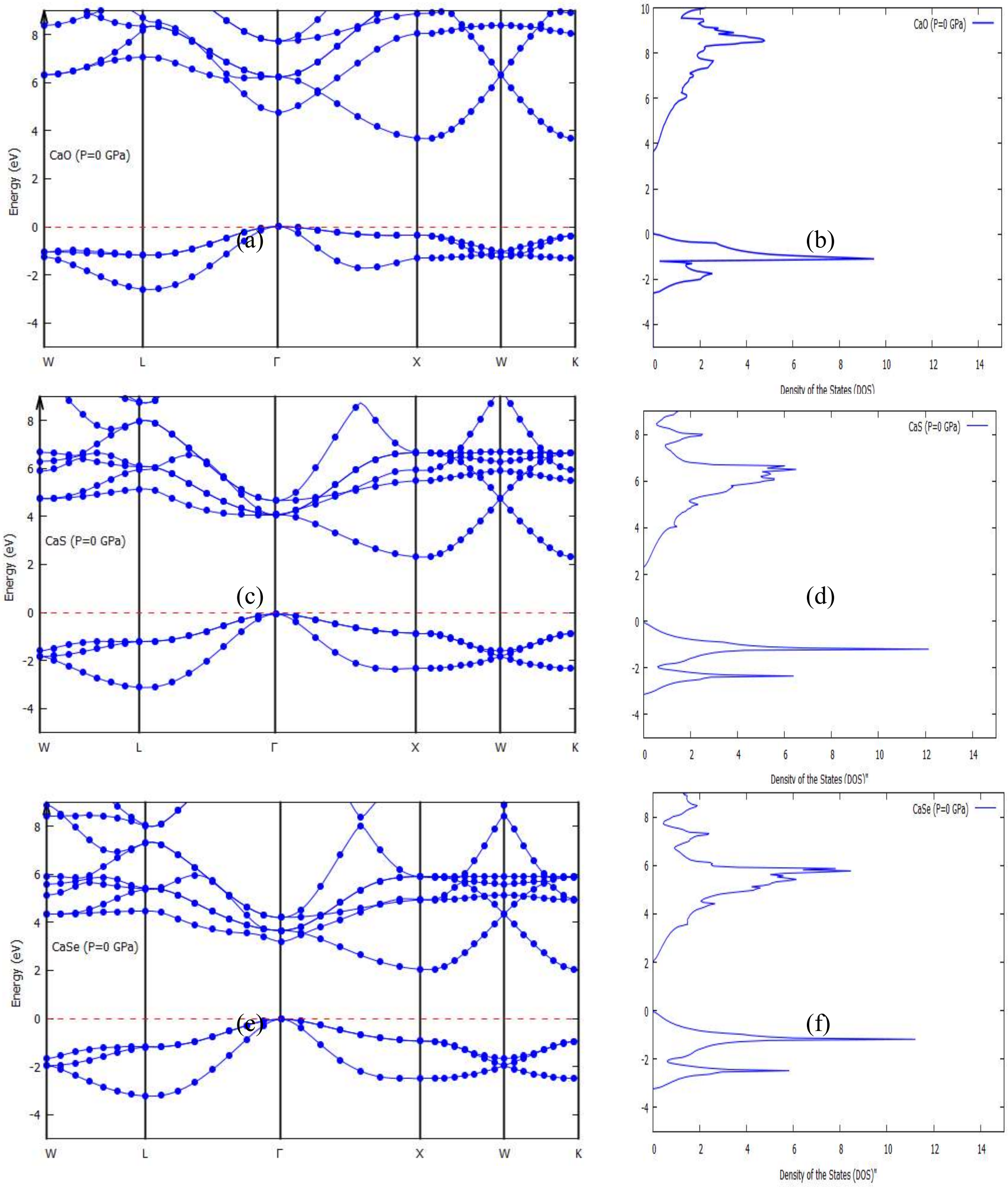


Figure 8: The equilibrium band structure and Density of the State (DOS) for Chalcogenides CaX (X=O, S, Se and Te) (a) and (b) is for CaO, (c) and (d) is for CaSwhere as (e) and (f) is for CaSe

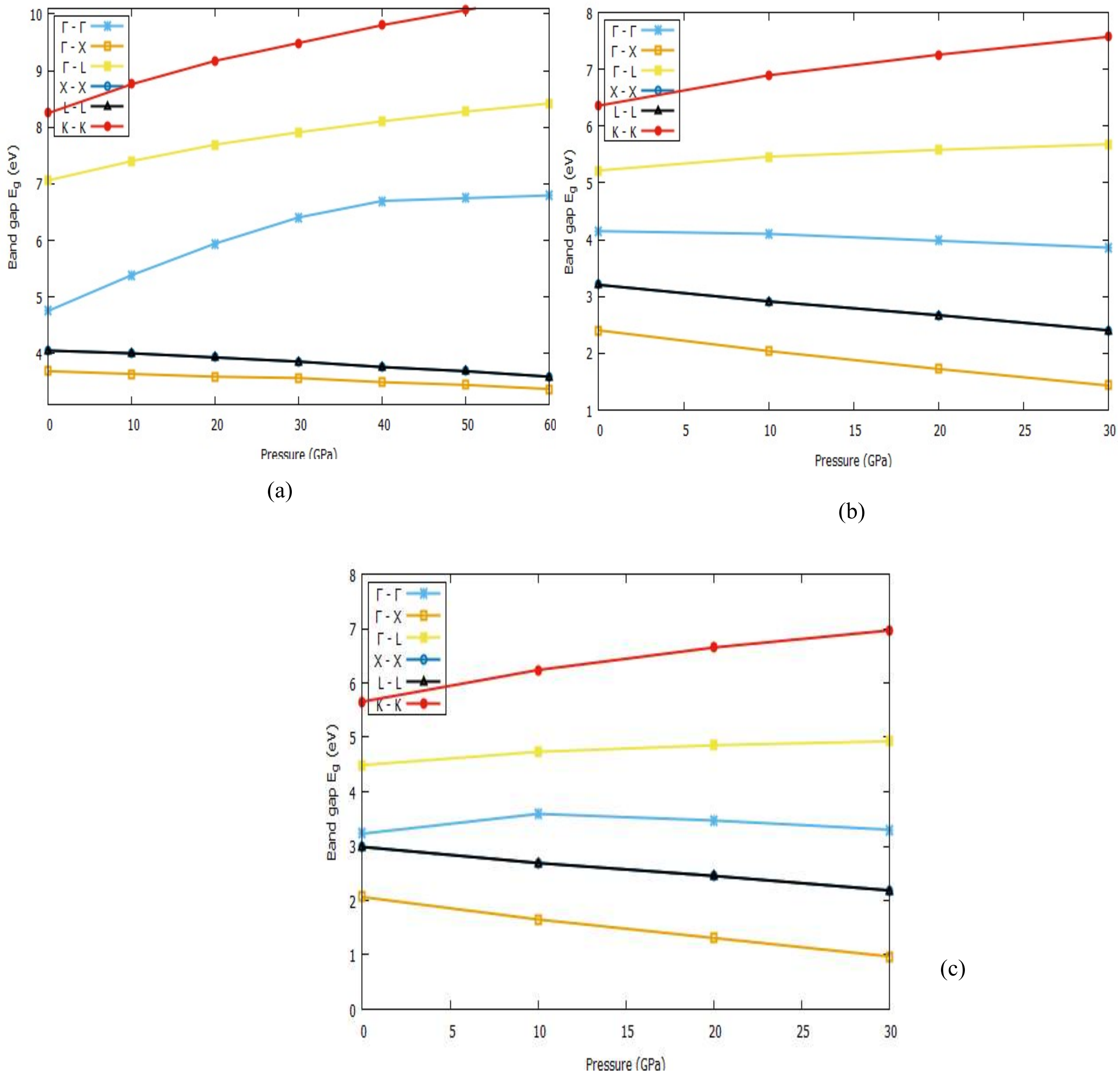
Table 3: Band gap for various pressure for CaX (X = O, S, Se) Chalcogenides for three pressure of 0 GPa, 40 GPa and 80 GPa

CaX		Pressure (GPa)	$(\Gamma - \Gamma)$ (eV)	$(X - \Gamma)$ (eV)	$(L - \Gamma)$ (eV)	$(X - X)$ (eV)	$(L - L)$ (eV)	$(K - K)$
CaO	This	0	4.76	3.69	7.06	4.05	8.25	4.1
	work	40	6.7	3.5	8.11	3.76	9.81	3.75
	Reference	80	6.87	3.28	8.69	3.42	10.75	3.45
CaS	This	0	4.15	2.4	5.22	3.2	6.36	3.2
	work	40	3.74	1.19	5.75	2.18	7.82	2.2
	Reference	80	3.2	0.27	5.81	1.31	8.52	1.4
CaSe	This	0	3.23	2.06	4.49	2.99	5.66	3.05
	work	40	3.16	0.68	4.93	1.94	7.23	2
	Reference	80	2.57	-0.34	5.02	1.02	8.01	1.1

Conclusion

Figure 10 shows the band-gap of the three compounds high symmetry point$(W - L - \Gamma - K - X - W - K)$The band-gaps at higher symmetry point $(K – K)$ increases with pressure,$(\Gamma - L)$almost constant except for the CaO which increase with pressure increase. For (L – L) and $(\Gamma - X)$the band-gaps decrease linear with pressure. Finally for the$(\Gamma - \Gamma)$decreases with pressure for CaS and CaSe.

At pressure of about 68GPa, CaSe undergoes phase transformation that is semiconductor-metal phase. At pressure of 80GPa all the three compounds became indirect band-gap material with minimum band-gap at$(\Gamma - X)$with values of 3.28eV, 0.27eV and -0.34eV for CaO, CaS and CaSe respectively.



(a)

(b)

(c)

Figure: Effect of pressure in Band gap at various symmetry point (G,X,L and K) for CaX (X=O, S and Se) (a) CaO, (b) CaS and (c) CaSe

Summary

We presented the effect of pressure on structural, mechanical and electronic properties of Chalcogenides CaX (X=O, S and Se) using density functional theory within generalized gradient approximation. We found out that:

- There is transition from B1 to B2 phase of these material, it was shown that, this material preferred been in B1 phase.
- There is collapse in the volume at transition pressure, the volume collapse were obtained to be 8.6%, 7.96% and 7.74% for CaO, CaS and CaSe respectively. This indicate that, the transition is first order transformation.
- The transition pressure were obtained to be 64.14, 38.33 and 35.71 for CaO, CaS and CaSe respectively. The transformation pressure decreases in the order CaO → CaS → CaSe, this can be attributed to the atomic weight of the compounds.
- At pressure of 29.8, CaSe is unstable and in all the B2 phases (CsCl) structure the compounds are not stable.
- The material moduli B, E and G increases with pressure linearly. The material are brittle at equilibrium, in which the degree of brittleness decreases with pressure. It was observed from the modulus ratio that these material became ductile at pressure of 50, 30 and 28. The degree of brittlity is in the order CaO → CaS → CaSe.
- Anisotropy of the material decrease and increase with pressure for B1 and B2 phases resepectively. CaO (B1) and CaS (B2) are Isotropic material at pressure of 12.5 and 97GPa respectively.
- The band-gap of these material CaO, CaS and CaSe, which are indirect band-gap semiconductors, with pressure measured at$(\Gamma - X)$are 3.69, 2.40 and 2.06eV. We observed that all the material (CaX) became indirect band-gap semiconductors at high pressure and the gap decrease with pressure increase.
- Finally, there is semiconductor-metal phase transition for CaSe at pressure 68 GPa.

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