Bulletin of Pure and Applied Sciences.
Vol.38 D (Physics), No.1, 2019: P.01-05

Print version ISSN 0970 6569
Online version ISSN 2320 3218
DOI: 10.5958/2320-3218.2019.00001.0

Original Research Article

Available online at www.bpasjournals.com

First Principles investigation of structural properties of CaX (X=S, Se, Te)

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Received on 18.01.2019 **Accepted on 07.04.2019**	

ABSTRACT In the present work, the first principle investigation of structural parameters of calcium chalcogenides in NaCl and CsCl structure using Linear Combination of Atomic Orbital (LCAO) method have been presented. In structural properties the lattice constant, bulk modulus and phase transition have been presented. Our results give the good agreement with previous theoretical and experimental data.

KEYWORDS Chalcogenides, NaCl, CsCl

INTRODUCTION

Calcium chalcogenides are having importance in industrial and technological applications, as they have large band gap. They have an important application for device modelling also. These compounds are thermionic materials. Also it can be used in magneto-optical devices. Among all the calcium chalcogenides CaSe has a special attraction, because this compound is having closed shell ionic systems at surrounding conditions that crystallizes in NaCl structure. Many experimental as well as theoretical studies have been done previously for calcium chalcogenides to investigate the structural properties and structural phase stability under pressure.[1] In the last decades the interest have been grown drastically to study the structural phase transition under the high pressure of calcium chalcogenides. As the insulator metal transition and the structural phase transition under high the high pressure produces the important theoretical predictions then the interest increased day by day. As calcium is belonging from group II and the chalcogenes are belonging from group VI of periodic table so when these two binary compounds makes the ternary compound like calcium chalcogenides it will form the II-VI semiconductor compound. Calcium sulphide has the chemical formula as CaS. It crystallizes in cubic rock salt structure. It also occurs as oldhamite in nature. In the presence of traces of heavy metals CaS becomes phosphorescent, like many other sulfides such as zinc sulfide or cadmium sulfide.It has a smell of rotten egg, which stems from H_2S formed by hydrolysis of calcium sulphide. [2] It is used as a sulfur based fertilizer. Calcium selenide (CaSe) is a chemical compound consisting of the elements calcium and selenium in equal stoichiometric ratio**.** In most of the volumes commonly the Calcium Selenied can be present. It is highly pure and is having the

submicron, nano-powder form.[3] Calcium telluride is a crystal grown product generally immediately available in most volumes. Calcium Telluride (CaTe) is also available as quantum dots. Calcium Telluride (CaTe) is also used in solar energy and advanced optical applications [4]. In view of this, it become mandatory and also worth full to study the structural properties of calcium chalcogenides compounds, thus in the present work the LCAO method as built in CRYTSAL [5] code has been used. The article is organized as follows: In section 2 we give a description of computational method. In section 3, result and discussions for structural properties are presented. Finally, the conclusion has been presented in section 4.

THEORETICAL DETAILS

In this work, the structural properties and the phase transition under the high pressure of CaX (X= S, Se, Te) have been investigated with the quantum mechanical simulation i.e. density functional theory (DFT). This method has proved to be efficient in many cases [6-7]. The function of hybrid scheme B3LYP has used inbuilt in crystal code. For the coding purpose, the Gaussian basis set have been used [8], The lattice constant and bulk modulus are computed for the B1 structure to B2 structure of CaS, CaSe and CaTe respectively.

RESULT AND DISCUSSIONS

The structural properties of the CaX(X=S,Se,Te) in rocksalt phase as well as in CsCl phase has been computed by calculating the total energy with the variation of volume of primitive cell of the crystal. In this work the phase transition under high pressure from rocksalt phase to CsCl phase of CaS compound has been showed in this work. Figure 1 and figure 2 represents the energy versus volume curve for the CaX(X=S,Se,Te) and figure 3 represents the first order phase transition from B1 to B2. In these figures, the dots represent the calculated energies through DFT and the curves represent the fitted energies to the Brich Mrughman equation of state.

$$E(V) = E_{\circ} + \frac{9V_{\circ}B_{\circ}}{16}\left\{\left[\left(\frac{V_{\circ}}{V}\right)^{\frac{2}{3}} - 1\right]^{3} B_{\circ}^{'} + \left[\left(\frac{V_{\circ}}{V}\right)^{\frac{2}{3}} - 1\right]^{2}\left[6 - 4\left(\frac{V_{\circ}}{V}\right)^{\frac{2}{3}}\right]\right\}$$

Where, E(V) represents the energy corresponds to the particular volume, E_o represents the equilibrium energy, V_o represents the corresponding volume, B_o is the pressure derivative of B.
The results are summarized in Table 1.

Table 1: Present and previously calculated lattice parameter (a), bulk modulus (B_0) for CaX (X= S, Se, Te).

	CaS(B1)	**CaS(B2)**	**CaSe(B1)**	**CaSe(B2)**	**CaTe(B1)**	**CaTe(B2)**
a (Å)						
Present	5.77	3.52	5.98	3.67	6.43	3.88
Experimental	5.689 [9]	3.46[9]	5.916[9]	3.611[9]	6.348[9]	3.931[9]
Other calculations	5.714[10]	3.487[10]	5.92[10]	3.62[10]	6.394[10]	3.917[10]
	5.717[11]	3.494[11]	5.968[11]	3.653[11]	6.396[11]	3.93[11]
B_0 (GPa)						
Present	57	59.23	47	52.15	37	39.23
Experimental	64[9]	64[9]	51[9]	51[9]	41.8[9]	41.8[9]

Other Calculations	57.7[10]	59.9[10]	48.56[10]	53.91[10]	39.22[10]	40.14[10]
	57.4[11]	60.7[11]	48.75[11]	51.41[11]	39.6[11]	38.78[11]
Phase transition from B1 to B2 in (GPa)						
	For CaS		For CaSe		For CaTe	
Present	31.88		30.5		27.12	
Experimental	40[9]		37.5[9]		33[9]	
Others Calculations	37.4[12]		35.1[13]		28.6[13]	
	36.5[12]		35.2[13]		30.2[13]	

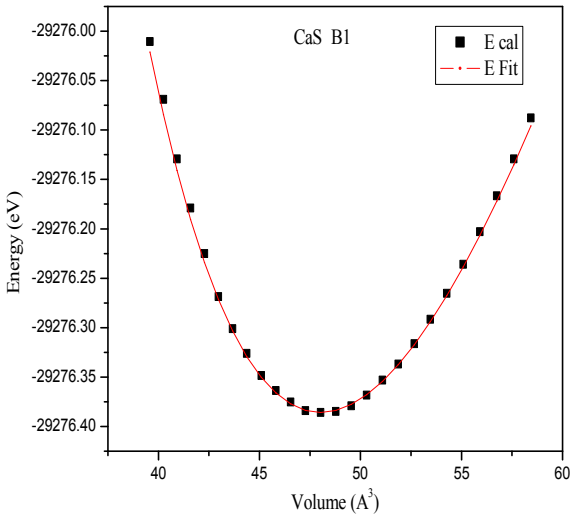

Figure 1:

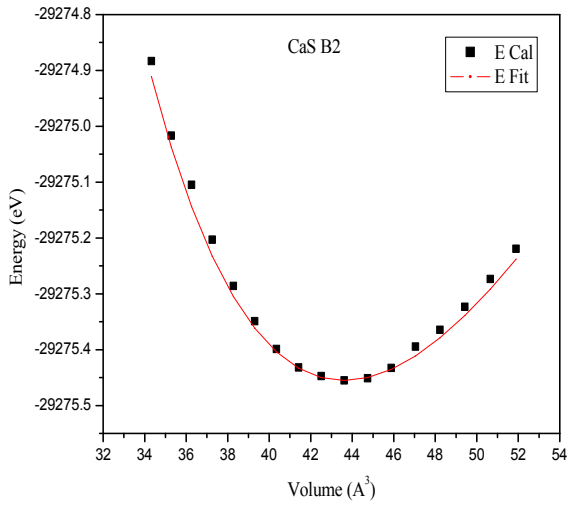

Figure 2:

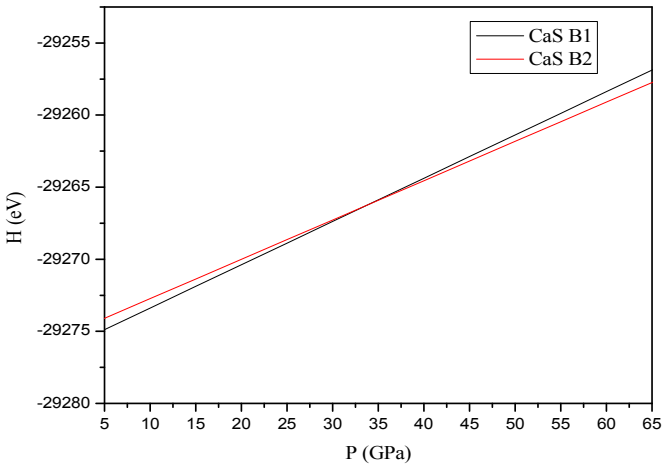

Figure 3:

CONCLUSION

In summary, LCAO method has been produced the result for the investigation of the structural properties of CaX where X is the chalcogenides compounds, that are sulfide, selenide, telluride. It has been observed that as the atomic mass of calcium chalcogenides compounds increases the lattice constant increases and bulk modulus decreases. It can also be concluded that CaS, CaSe, CaTe undergo structural phase transition from B1 to B2 phase under high pressure. Also it has been observed that the phase transition for CaS, CaSe and CaTe at a pressure at a pressure of 31.88, 30.5 and 27.12 GPa respectively. Present results are consistent with previous investigations.

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