FIRST PRINCIPLE STUDIES ON CALCIUM CHALCOGENIDE, CaSe FOR THE DETERMINATION OF STRUCTURAL AND ELECTRONIC PROPERTIES

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Abstract

In the present work, we report an investigation on the structural and electronic properties of II–VI semiconductor compounds (alkaline-earth chalcogenides), CaSe, using First-Priniciples calculations performed using the local density approximation (LDA) and the PBE generalized gradient approximations for the exchange-correlation functional using QUANTUM ESPRESSO. The lattice parameters of the structures were obtained by total energy minimization of the crystal. The equilibrium lattice constant for CaSe compound agrees well with the experimental result. The alkaline-earth chalcogenides ,CaSe form an important closed-shell ionic system in the NaCl-type structure at ambient conditions. The obtained band structure calculations suggest that the CaSe compound are semiconductors at 0 GPa, is in good agreement with literature available. The present results of CaSe are in excellent agreement with experimental works available.

Keywords: *Quantum Espresso, Electronic Structure, Structural Properties, Band Gap, First Principle Calculations*

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1. INTRODUCTION

The II–VI semiconductor compounds, alkaline-earth chalcogenides, are obtained from group II and VI elements of the Periodic Table.

These alkaline-earth chalcogenides form an important group of semiconductors with a large band gap. Because of their large gap, they constitute an important set of materials from technological point of view. So, the studies of their electronic structure are of huge interest in device modelling. They are used as a material for a numerous applications like magneto-optical devices. These compounds are thermionic materials. Among these compounds, in recent years, the alkaline-earth chalcogenides, (CaSe) have attracted a special attention.

The CaSe compounds form an important family of closed-shell ionic systems at ambient conditions that crystallize in the NaCl , six-fold structure.

Density Functional theory related studies of the structural and electronic properties of semiconducting materials are done by means of first principle studies. These methods allow us to obtain the total energy of the system to accurate values, under local density approximation.

In the present work, we put forward a systematic study of the structural properties, electronic properties using the local density approximation (LDA) and PW91 based gradient approximations for the exchange-correlation functional using QUANTUM ESPRESSO (open source).

The rest of the paper is presented as follows. In the section 2, we mention about the methods that we have followed, In Section 3, we present and discuss our results, and also comparing them with the literature, in Section 4, we present the conclusions from the current work.

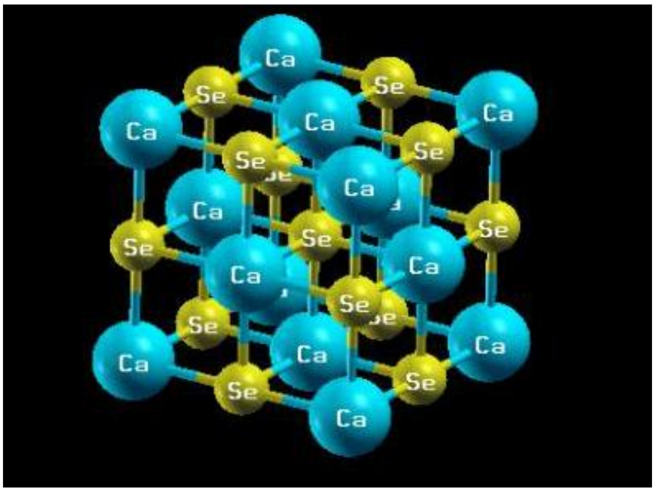

Fig.1 Case Structure (as seen in XcrysDen)

2. COMPUTATIONAL METHODS

We use the QUANTUM ESPRESSO (1) which is a computer package to study the electronic structure and optimization using the molecular dynamics simulation. The Quantum ESPRESSO distribution contains the main packages PWscf (Plane-Wave Self-Consistent Field) for obtaining electronic-structure properties by Density-Functional Theory (DFT), using a Plane-Wave (PW) basis set and pseudopotentials. It has in it more packages for specific purpose calculations.

We have also used XCrySDen (2) which is a molecular-structure visualisation program based on the crystalline structure. The XCrySDen acronym stands for Crystalline Structures and Densities and X since it is suitable for X-Window environment. It facilitates a display of iso-surfaces and contours, which can be seen as crystalline structures and for better visualization, interactive rotation too is provided as a part of the same program. The Structure of CaSe can be seen in Figure (1).

In order to calculate the ground state properties of CaSe, the total energies are calculated in the NaCl-type structure , The cutoff energy is calculated first and then the lattice parameter is obtained by total energy minimization of the crystal.

3. RESULTS AND DISCUSSION

3.1 Structural Properties of Case

Now we will study the structural properties of CaSe. At ambient conditions without the application of any external pressure, CaSe would be in the NaCl (B1) phase.

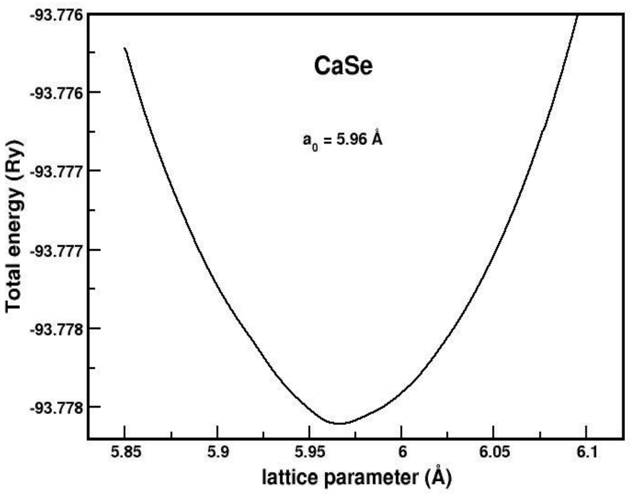

Fig-2 Lattice Parameter

After obtaining the cutoff energy after a few computations, the method of minimizing the total energy of the crystal was followed to obtain the lattice parameter value of CaSe. The same is plotted in Fig-2.

At ambient conditions ,it is seen that the NaCl (B1) phase is the stable structure for CaSe, which is in good agreement with the experimental and also theoretical results. The current lattice parameters obtained in the NaCl (B1) structure is 5.96 Å.

3.1 Electronic Properties of Case

Fig - 3 shows the electronic energy band structure calculated at ambient pressure for CaSe compounds at the high-symmetry points in the Brillouin zone. Here for reference, the top of the valence band is considered as zero energy.
The CaSe is actually a direct band-gap semiconductor in NaCl (B1) structure at ambient pressure.

The Band gap energy is calculated to be 2.86 eV as can be observed from Fig 3.

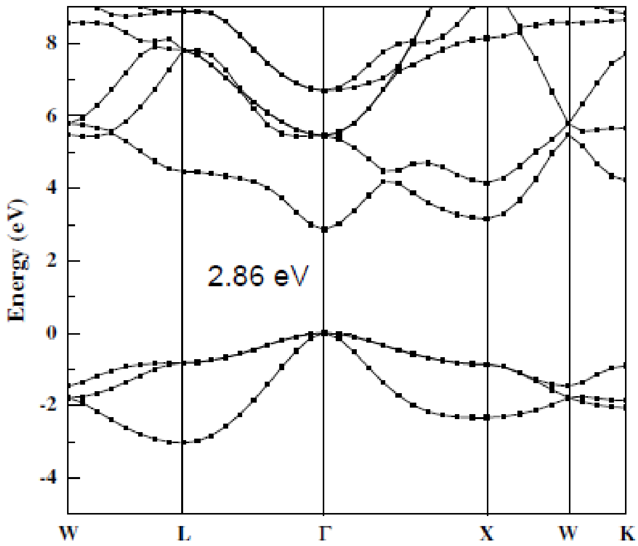

Fig 3 - Band Structure of CaSe

4. CONCLUSIONS

To conclude, we have done an investigation on the structural properties of CaSe using First-Priniciples calculations and we compare our result with the available experimental results (3) and with the earlier theoretical works (4) and it can be clearly observed that the results in this present work are in well agreement with the published results.

The calculated equilibrium lattice constant (*a*0) of CaSe in the present work it is 5.96 Å and by by experimental work it is 5.97 Å and by other theoretical works is 5.968 Å.

From the Electronic band structure obtained, we conclude that CaSe is a direct band gap semiconductor with an obtained value for band gap of 2.86 eV.

Table -1: Calculated equilibrium lattice constant of CaSe and comparison

a0 (lattice constant) (Å)	Present Work (Å)	Experimental Work (Å)	Other Theoretical works (Å)
CaSe	5.96	5.97 (3)	5.968(4)

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