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Ab initio study for Structural and Electronic properties of Rock Salt CaS

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Abstract - *In the current work, we perform an ab-initio study of structural and electronic properties of CaS using density functional theory with the plane wave basis set as implemented in the QUANTUM ESPRESSO code. The lattice parameter of the structure was obtained by minimizing the total energy of the crystal. The equilibrium lattice constant for CaS compound agrees well with the experimental result. The electronic band structure calculations suggest that the CaS compound is a direct band gap semiconductor at ambient pressure, and is in good agreement with literature data. The present structural and electronic parameters of CaS agree well with the available experimental work*

Key Words: Density Functional Theory, Electronic Properties, Quantum Espresso

1. INTRODUCTION

The II–VI semiconductor compounds are made from group II and VI elements of the Periodic Table. Because of their large gap, they are important materials from technological point of view. They are used as a material for various applications like magneto-optical devices. These compounds are thermionic materials. So, the studies of their electronic structure are of huge interest in device modelling. These compounds (II–VI) (CaS) form a very important group of semiconductors with a large band gap.

The II–VI semiconductor compounds (CaS) form an important family of closed-shell ionic systems that crystallize in the six-fold coordinated NaCl (B1) structure at ambient conditions.

Theoretical studies of the structural and electronic properties of semiconducting materials are performed by means of ab initio calculations. These methods allow us to obtain with great accuracy the total energy of the system, usually using the density functional theory, DFT, under local density approximation, LDA.

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

The rest of the paper is organized as follows. In 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.

2. 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 core packages PWscf (Plane-Wave Self-Consistent Field) and CP (Car-Parrinello) for the calculation of electronic-structure properties within Density-Functional Theory (DFT), using a Plane-Wave (PW) basis set and pseudopotentials.

We have also used XCrySDen [2] which is a crystalline- and molecular-structure visualisation program. The name of the program stands for Crystalline Structures and Densities and X because it runs under the X-Window environment. It facilitates a display of iso-surfaces and contours, which can be superimposed on crystalline structures and interactively rotated and manipulated. The Structure of CaS can be seen in Figure-1

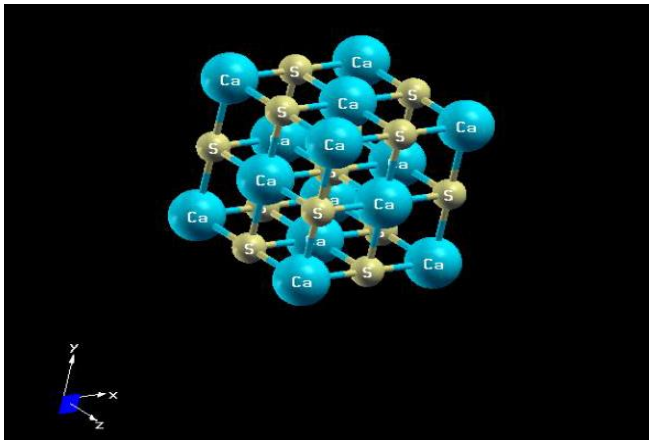

Figure- 1 CaS Structure (XcrySDen)

In order to calculate the ground state properties of CaS, the total energies are calculated in the rocksalt structure.

The cutoff energy is calculated first and then the lattice parameter is obtained by minimizing the total energy of the crystal.

We perform calculations of the total energy of CaS in the six-fold B1, rocksalt structure in order to obtain the lattice parameter.

3. RESULTS AND DISCUSSION

3.1 Structural Properties

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

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The Cutoff energy is obtained for CaS and can be observed from the Figure 2 provided below.

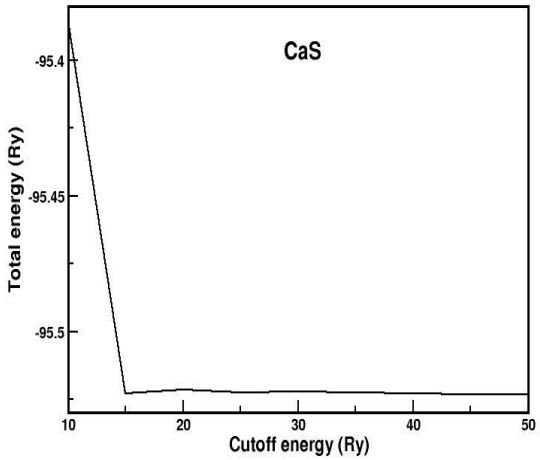


Figure - 2 Cutoff Energy

Once the cutoff energy is obtained, then the method of minimizing the total energy of the crystal was followed to obtain the lattice parameter value of CaS. The same is plotted in Figure-3.

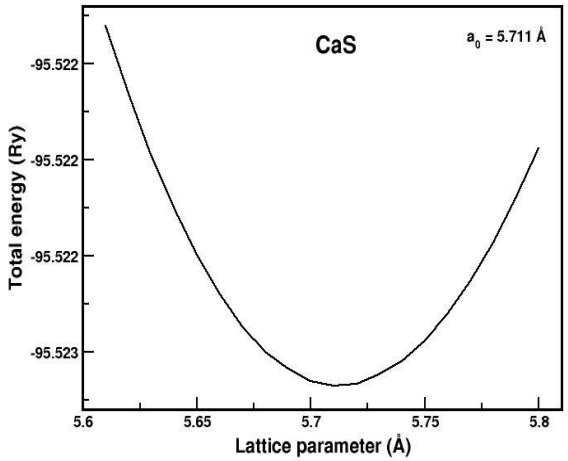


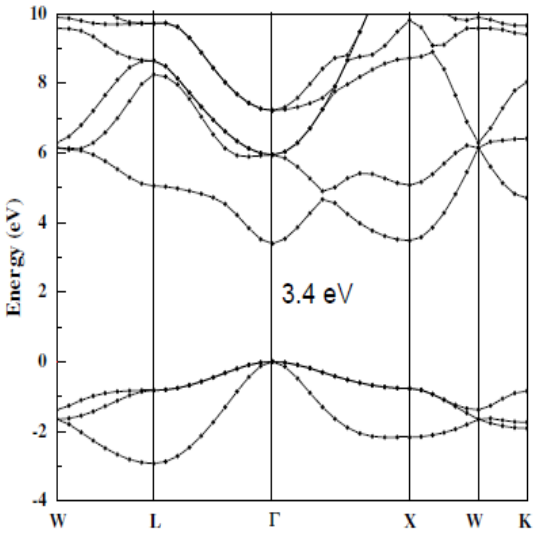
Figure -3 Calculation of Lattice Parameter

It is seen that the rock-salt (B1) phase is the stable structure at ambient conditions for all compounds, which is consistent with the experimental and other theoretical results. The present lattice parameters computed the rock-salt (B1) phase structure is 5.711 Å.

3.2 Electronic Properties

Here, Figure - 4 shows the electronic energy band structure calculated for rocksalt phase of CaS compound at the high-symmetry points in the Brillouin zone at ambient pressure. Here the top of the valence band is taken as zero energy.

The CaS is direct band-gap semiconductor in (B1) Phase, with the minimum conduction band and the maximum valence band at the mid point. The energy gap is found to



occur between the chalcogen p bands and the Calcium 3d-bands.

The Band gap energy is calculated to be 3.4 eV.

Figure – 4 Electronic Band Structure in CaS

4. CONCLUSIONS

To conclude, we have done an investigation on the structural properties of CaS using First-Priniciples calculations and we compare our result with the available experimental results [3] and the previous theoretical data [4] and it can be clearly observed that the results in this present work are in well agreement with the experimental results..

The calculated equilibrium lattice constant ($a0$) of CaS in the present work it is 5.711 Å and by by experimental work it is 5.714 Å and by other theoretical works is 5.717 Å

From the Electronic band structure obtained, we conclude that CaS is a direct band gap semiconductor with a band gap of 3.4eV.

Table-1: Calculated equilibrium lattice constant ($a0$ in Å) of CaS and comparison

a0 (lattice constant) (Å)	Present Work (Å)	Experimental Work (Å)	Other Theoretical works (Å)
CaS	5.711	5.714 (3)	5.717 (4)

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REFERENCES

[1] P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009); URL http://www.quantum-espresso.org

[2] Kokalj: J. Mol. Graphics Modelling, 1999, Vol. 17, 176--179. Code available from http://www.xcrysden.org.

[3] H. Luo, R.G. Greene, K. Ghandehari, T. Li, and A.L. Ruoff, Structural phase transformations and the equations of state of calcium chalcogenides at high pressure, Phys. Rev. B 50 (1994), pp. 16232–16237.

[4] Z. Charifi, H. Baaziz, F. El Haj Hassan, and N. Bouarissa, High pressure study of structural and electronic properties of calcium chalcogenides, J. Phys. Condens. Matter 17 (2005), pp. 4083–4092