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First-principles calculations to investigate the structural and electonic properties of $CaSiO_3$.

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Abstract

As an alternative to traditional photovoltaic semiconductors, perovskite materials like ABX_3 have recently caught the interest of researchers. These materials unique physical traits and specific gap values, which have a significant impact on their overall effectiveness and performance, are what essentially led to this shift in attention. Using the ab initio method calculations. The structural and electrical characteristics of $CaSiO_3$, a tetragonal compound, are investigated in this work using first-principles calculations based on the full potential-linearized augmented plane wave technique (FP-LAPW) within the density functional theory (DFT). Our study thoroughly examines electrical properties, such as band structure and density of states (DOS), to predict $CaSiO_3$ viability as a potential photovoltaic material. $CaSiO_3$ is a promising candidate for future exploration because preliminary results indicate that it exhibits semiconductor properties.

Key- Words:

Ab initio, Perovskite, first principal, FP-LAPW, DFT.

Introduction

The general formula of perovskite is ABX_3. This structure gives perovskites unique electronic and magnetic properties, which make them promising materials for a wide range of applications. The tetragonal form has attracted significant attention in recent years due to its potential applications in a wide range of fields.

Method of Calculations

The total energies were calculated within the full potential linearized augmented plane wave (FPLAPW) +local orbitals (lo) method, implemented in the WIEN2K code [1]. In addition to its accuracy and reliability. In order to investigate structural, electronic properties, the FP-LAPW method is used [2], under the purview of the density functional theory (DFT) as executed in Wien2k code [3].

We used the GGA13 approximation, which is a type of exchange-correlation functional that is often used in ab initio calculations. GGA13 is a specific type of GGA functional that was developed by Perdew and co-workers in 2013 [4]. We use a k-mesh of 2000 points.

Structural properties

The calculated total energy versus volume are fitted to the Murnaghan's equation of state [5]. Figure 2 presents the plot of total energy as a function of volume for this compound in the structure phase with space group P4/mbm. The lattice parameter that has been optimized using the volume with the lowest total energy is equal to a = 9.638 Å and c = 6.858. This lattice parameter was used in the second part to calculate the other properties. The compound has a bulk modulus of approximately 214.8083 GPa.

	a = b (bohr)	c (bohr)	B (GPa)	B'
$CaSIO_3$	9.638	6.858	214.8083	4.475

Table 1 : Lattice constant a, bulk modulus B, pressure derivative of bulk modulus B′, and elastic constants parameters of $CaSiO_3$ at zero pressure and zero temperature.

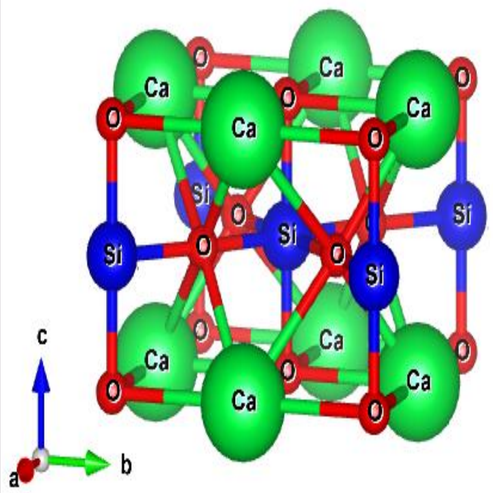

Figure 1: Crystal structure of $CaSiO_3$ in tetragonal phase.

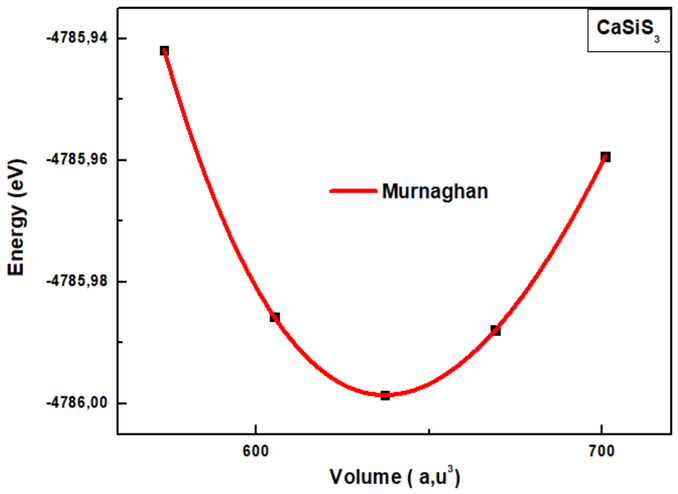

Figure 2: Total energy as a function of the volume for states of $CaiIO_3$ in the P4/mbm structure.

Electronic properties

The FP-LAPW method was utilized to compute its energy band structure and both the TDOS and PDOS. Figure 3 shows that the valance band is mainly a result of the O(p) states, while the contribution band originates from the Si(s/p) states. with a small contribution from Ca(s/p) states. Figure 4 shows indirect gap for the $CaSiS_3$, where the valance band maximum is located at Γ and the conduction band minimum at Z

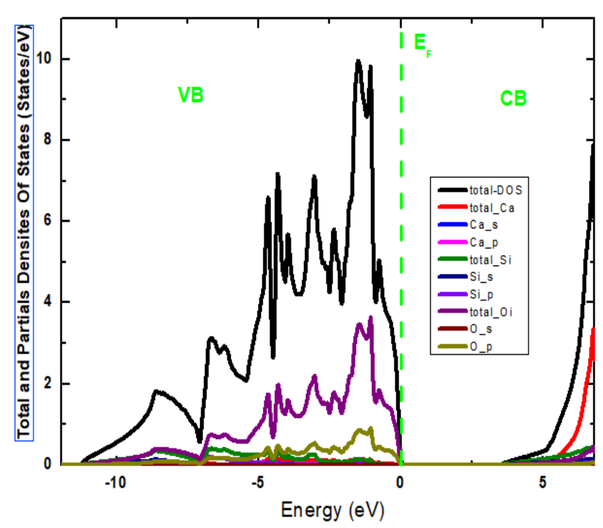

Figure 3: Total energy as a function of the volume for states of $CaSiO_3$ in the P4/mbm structure.

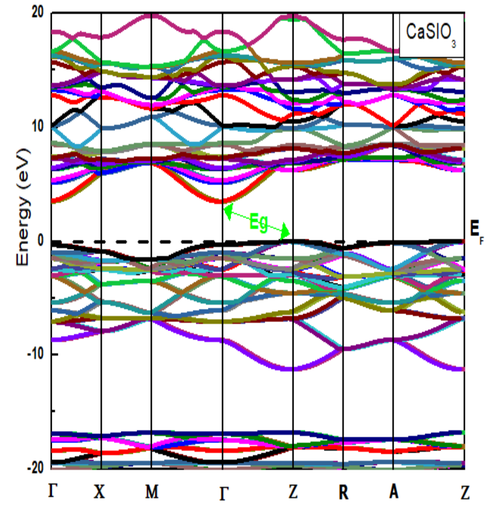

Figure 4: Electronic band structure of cubic $CaSiS_3$

Conclusion

In this work, we performed a first-principles calculation to determine the structural and electronic properties of $CaSiS_3$ using the GGA approximation. Our results showed that the lattice parameters were calculated in a good tetragonal arrangement. The band structure showed that the compound has semiconductor behavior

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