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Exploring the Structural and Electronic Properties of CaZnX (X = C and Si) Half-Heusler Compounds: A DFT Investigation

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ABSTRACT

This study employs Density Functional Theory in WIEN2k software to investigate the structural and electronic parameters of CaZnX (X = C and Si) half-Heusler materials. The Perdew-Burke-Enzerhof (PBE-GGA) potential functional, was utilized for structural optimization and the Tran-Blaha modified Becke and Johnson (TB-mBJ) approach is incorporated with PBE-GGA for band gap and optical parameters determination. The investigation of these materials reveals correlations between their atomic composition and lattice dimensions, as well as their semiconductor behavior.

***Keywords**: Half-Heusler, Lattice Constant, Bulk Modulus, Band Structure.*

Introduction

In recent years, the escalating rate of carbon emissions has become a pressing global concern, posing a significant threat to the environment. To address these environmental challenges, there's a critical need for materials that can function as both photovoltaics and thermoelectric generators. Researchers have explored a wide array of materials for photovoltaic and thermoelectric applications **[1-8]**. Among these materials, half-Heusler compounds have garnered considerable attention due to their extensive range of potential applications, straightforward crystalline structure, and intriguing properties. Originating from the foundational discovery of Heusler alloys in 1903 by Fredrich Heusler**[9]**, these materials have evolved to occupy a significant niche in the scientific landscape.

Gruhn **[10]** investigated tailored semiconductor materials for optoelectronic applications like thin-film solar cells and laser diodes. He analyzed 648 ternary 1:1:1 half-Heusler compounds using ab initio calculations, uncovering preferred configurations and trends in semiconductivity. Using DFT, Azouaoui et al. **[11]** examined the structural and physical properties of NaCaZ (Z= N, P, As) half-Heusler (HH) semiconductor materials under pressures up to 20GPa. The results revealed their chemical stability in the α-phase structure, along with semiconducting behavior characterized by an indirect bandgap and promising optical properties. Wu et al. **[12]** conducted first-principles calculations to examine the effects of pressure on NaAlSi's mechanical and dynamical stability. They observed a decrease in lattice constants and an increase in elastic constants under pressure, with mechanical instability occurring when C_{44} decreases above 25.97 GPa. Phonon-dispersion curves suggested structural stability at ambient pressure but predicted instability beyond 27.52 GPa, indicating a potential phase transition. Jin et al. **[13]** explored the topological band structure of NaAlSi, revealing four type-I nodal lines near the Fermi level and identifying drumhead surface states. Yi et al. **[14]** proposed NaAlSi(Ge) as dual double node-line semimetals with unconventional surface states, suitable for studying correlated phases and as cathode materials for sodium-ion batteries. Yasemin O. Ciftci's **[15]** ab-initio study confirmed NaAlSi's mechanical stability as a semiconductor with potential for optoelectronic applications. Wang et al. **[16]** investigated NaAlGe, identifying it as a topological nodal line semimetal with distinct surface states, suitable for electronic devices. These studies collectively showcase the diverse properties and potential applications of these materials.

The literature review underscores a notable lack of investigation into Ca-based half-Heusler materials. This observation serves as a motivating factor for the research endeavors, prompting a comprehensive exploration into the structural and electronic characteristics of CaZnC and CaZnSi half-

Heusler compounds. This study aims to determine the potential suitability of these materials for incorporation into renewable energy devices.

Research Methodology

The investigation of structural and electronic parameters of the selected materials was conducted using WIEN2k software**[17, 18]**.The cutoff energy for calculations was set at -6.0 Ry. The atomic sphere expansion of the spherical harmonics was set to l_{max} = 10 to ensure adequate representation of electronic states. The value of $R_{MT}K_{max}$ was set to 7.0 for both compounds. G_{max} was set to 12 to ensure convergence and accuracy in the calculations. The structural optimization was done to compute various parameters using a generalized gradient approximation based on the Perdew-Burke-Enzerhof (PBE-GGA) configuration**[19]**. Since PBE-GGA underestimates the band gap, hence in pursuit of a more precise band gap value, the researchers employed the Tran-Blaha modified Becke and Johnson (TB-mBJ) approach**[20]** in addition to the PBE-GGA method. A 10×10×10 k-mesh was utilized in the first Brillouin zone for calculating the various parameters.

Results and Discussion

- **Structural Properties**

CaZnX (X = C and Si)half-Heusler materials exhibit crystalline structures belonging to the F-43m space group. The unit cell structures of these investigated materials are illustrated in Figure 1.

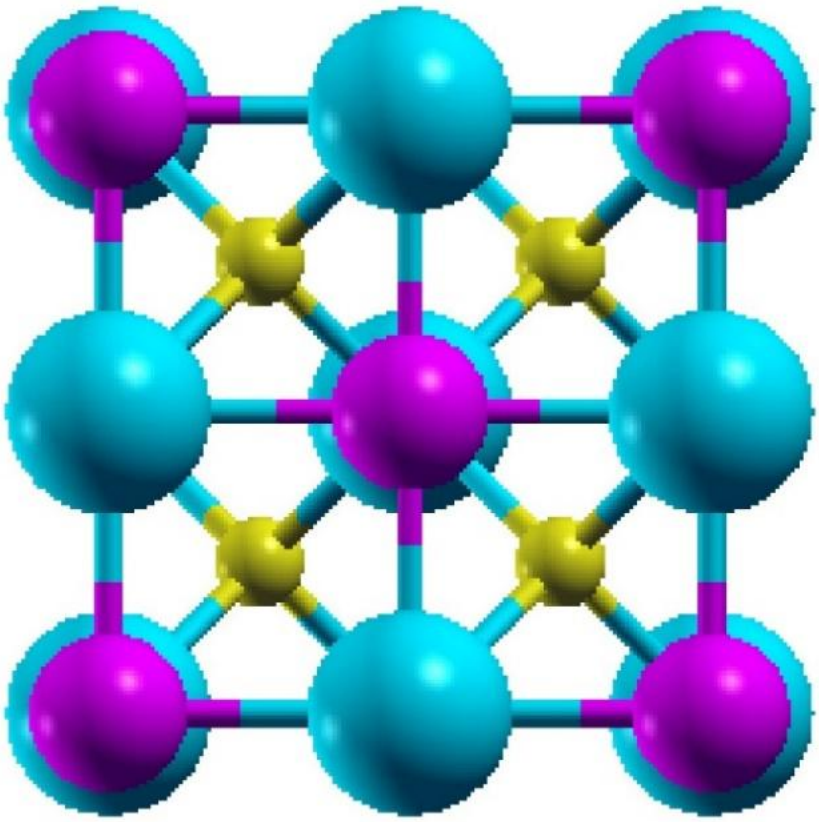

Figure 1: The unit cell of CaZnX (X = C and Si) HH Compounds. Cyan color denotes Ca-atom, magenta color denotes Zn-atom, and yellow color denotes X-atom.

Figure 2 illustrate the energy-volume graphs of the studied materials. Through this analysis, various structural parameters, including equilibrium energy ('E' in Ry), lattice constant ('a' in Å), bulk modulus ('B_0' in GPa) at zero pressure, and its first pressure derivative (B_0'), were determined.

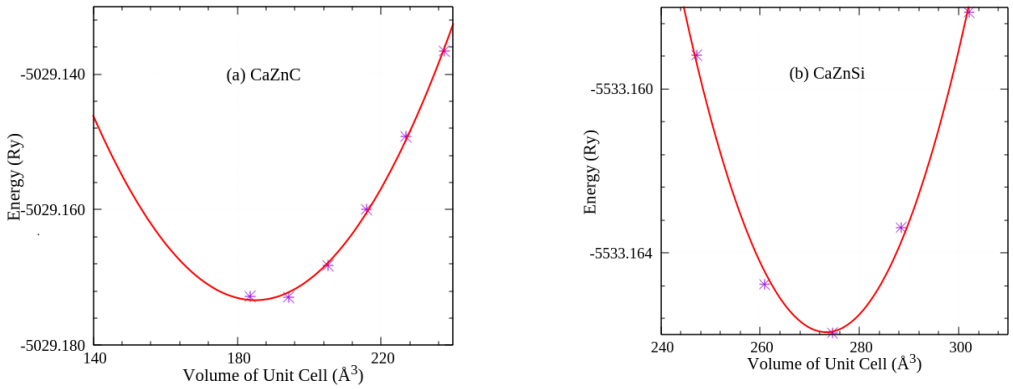

Figure 2: Volume optimization curve of (a)CaZnC and (b)CaZnSi HH compounds.

The lattice constant of CaZnC and CaZnSi was observed to be 5.7Å and 6.4Å respectively. The bulk modulus of these materials was observed to be78 GPa and 47 GpParespectively, i.e., it exhibits an inverse trend compared to that of the lattice constants. Moreover, a compound's thermoplastic qualities can be inferred from the pressure derivative of bulk modulus.For every material used in this investigation, the pressure derivative of bulk modulus was found to be positive, suggesting that these substances had a tendency to become more rigid with increasing pressure.

- **Electronic Properties**

The self-consistent field (SCF) calculations were performed using the Perdew-Burke-Enzerhof (PBE-GGA) potential functional with optimized lattice parameters. It was observed that CaZnC exhibited a low band gap, while CaZnSi exhibited zero band gap. This phenomenon may arise due to the underestimation of band gaps by PBE-GGA potential, as noted in earlier studies**[21, 22]**. To address this, the researchers applied the Tran-Blaha modified Becke and Johnson (TB-mBJ) approach to modify the results obtained from the PBE-GGA potential functional. This approach adjusts certain input parameters of the semi-local potentials, aiming to reproduce band gaps closer to experimental values **[23]**. After applying TB-mBJ the band gap of CaZnC and CaZnSi was to be 1.1 eV and 1.0 eV respectively. Figure 3 illustrates the band structure curves of these materials under ambient pressure conditions. Analysis of Figures 3(a) &3(b) reveals a notable characteristic: CaZnC exhibits direct band gap, while CaZnSi exhibits indirect band gap.

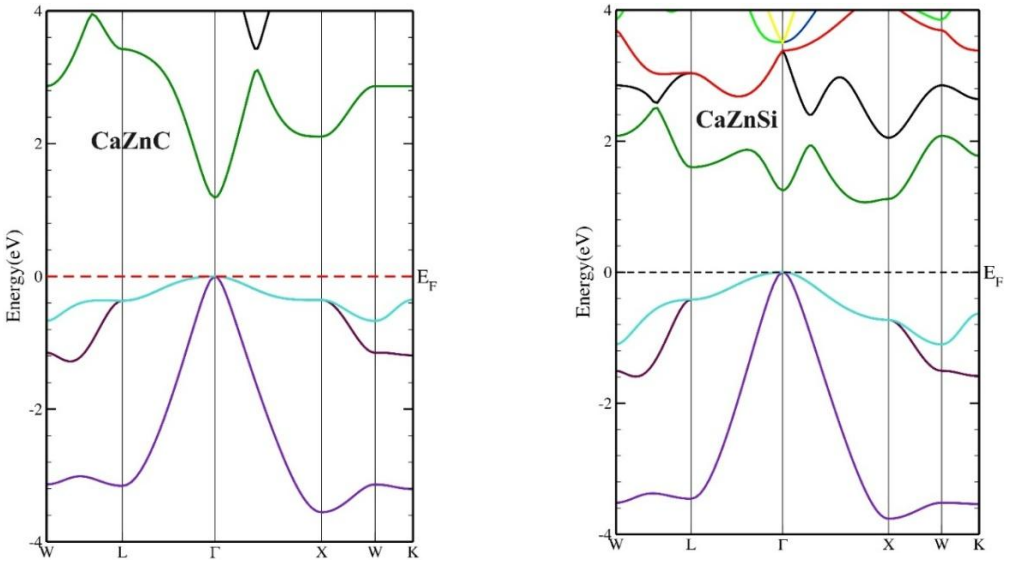

Figure 3: Band structure plots of (a)CaZnC and (b)CaZnSi HH compounds.

Conclusion

This comprehensive study explores the diverse properties of CaZnX (X = C and Si) half-Heusler materials. Lattice constants were determined as 5.7 Å for CaZnC and 6.4 Å for CaZnSi, with CaZnSi exhibiting greater compressibility. Both materials manifest semiconductor behavior, with band gaps measured at 1.1 eV for CaZnC and 1.0 eV for CaZnSi. These findings underscore the materials' versatility for various technological applications, guiding future research in materials science and engineering.

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