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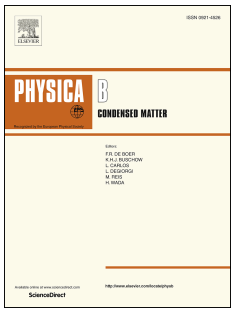

Structural, electronic, elastic, and thermodynamic properties of CaSi, Ca_2Si, and $CaSi_2$ phases from first-principles calculations

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Structural, electronic, elastic, and thermodynamic properties of CaSi, Ca_2Si, and $CaSi_2$ phases from first-principles calculations

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Abstract: The structural, electronic, elastic, and thermodynamic properties of CaSi, Ca_2Si, and $CaSi_2$ are systematically investigated by using first-principles calculations method based on density functional theory (DFT). The calculated formation enthalpies and cohesive energies show that $CaSi_2$ possesses the greatest structural stability and CaSi has the strongest alloying ability. The structural stability of the three phases is compared according to electronic structures. Further analysis on electronic structures indicates that the bonding of these phases exhibits the combinations of metallic, covalent, and ionic bonds. The elastic constants are calculated, and the bulk modulus, shear modulus, Young's modulus, Poisson's ratio, and anisotropy factor of polycrystalline materials are deduced. Additionally, the thermodynamic properties were theoretically predicted and discussed.

Keywords: First-principles calculations; Electronic structures; Elastic constants; Thermodynamic properties

1. Introduction

The Ca-Si intermetallic compounds including CaSi, Ca_2Si, and $CaSi_2$ are composed of inexpensive elements and are widely used in energy, aerospace, electronics, and other fields [1–4]. These compounds have several unique properties, CaSi can be used as a hydrogen storage material because H atoms can be easily absorb onto its surface, creating $CaSiH_3$ [5]. Ca_2Si is an environment-friendly semiconductor, with a 1.9-eV band gap at room temperature, which can be used for photoelectric and thermoelectric conversion [6]. The 6R structure of $CaSi_2$ was discovered by Kautsky in the 1950s [7]. $CaSi_2$ particles, which can be formed in Si-containing magnesium alloys by adding Ca into the melt, can act as heterogeneous nuclei of Mg_2Si phases, modifying their morphology [8]. In addition, $CaSi_2$ particles have good thermal stability and thus enhance the heat-resistant capability of magnesium alloys.

The thermodynamic data of Ca-Si intermetallic compounds are still incomplete [9,10], and making it important to systematically investigate their various properties. In this work, we carried out first-principles calculations to investigate the electronic, elastic, and thermodynamic properties of CaSi, Ca_2Si, and $CaSi_2$ phases, in order to evaluate their structural and thermal stability.

2. Computational methods

Calculations of the total energy and electronic, elastic, and thermodynamic properties were performed with the Cambridge sequential total energy package (CASTEP), a first-principles plane-wave pseudopotential based on density functional theory (DFT) [11]. The

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