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Electronic, elastic, and thermodynamic properties of complex hydrides XAlSiH (X = Sr, Ca, and Ba) intended for hydrogen storage: an *ab-initio* study

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Abstract

The mechanical and thermodynamic properties of polyanionic hydrides XAlSiH (X = Sr, Ca, and Ba) were evaluated using density functional theory (DFT). The thermal parameters of XAlSiH hydrides, such as the Grüneisen parameter γ, heat capacity, and thermal expansion coefficient, were computed for the first time. The quasi-harmonic Debye model was used to determine these parameters over a range of pressures (0–40 GPa) and temperatures (0–1000 K). The gravimetric hydrogen storage capacities for BaAlSiH, SrAlSiH, and CaAlSiH were found to be 0.52%, 0.71%, and 1.05%, respectively. The hydrogen desorption temperatures for these compounds were also simulated at 748.90 K, 311.57 K, and 685.40 K. Furthermore, semiconducting behavior with an indirect bandgap value between 0.2 and 0.7 eV was exhibited by these compounds using the GGA and LDA approximation, and between 0.7 and 1.2 eV using the mBJ-GGA and mBJ-LDA approximation. Accurate elastic constants for single crystals were obtained from the calculated stress–strain relationships. The elastic constants for the XAlSiH compounds were significantly higher than those for other hydrides. The [001] direction was more compressible than the [100] direction in the hexagonal structure of XAlSiH. A lower bulk modulus than metallic hydrides was exhibited by these materials, indicating that XAlSiH compounds (X = Sr, Ca, and Ba) were highly compressible. The melting temperature for CaAlSiH was higher than that for SrAlSiH and BaAlSiH. Consequently, the decomposition temperature for XAlSiH (X = Sr and Ba) at which hydrogen was released from a fuel cell was lower than that for CaAlSiH. The bonding behavior of CaAlSiH was more directional than that of SrAlSiH and BaAlSiH. Brittle materials were XAlSiH (X = Sr, Ca, and Ba). Our PBE calculations yield linear compressibility and orientation-dependent Young's modulus. Materials composed of hexagonal XAlSiH (where X represents Sr, Ca, or Ba elements) exhibit anisotropy in Young's modulus but isotropy in bulk modulus.

1. Introduction

In recent times, there has been extensive research on renewable energy sources as a result of the constraints posed by finite energy resources including oil, coal, and gasoline [1, 2]. The primary issue associated with utilizing renewable energy sources for powering automobiles is the inherent inefficiency of the processes involved [3, 4]. Hydrogen energy is considered a promising alternative due to its abundant and inexhaustible source [5–7]. Nevertheless, the direct compression of hydrogen gas into the tank resulted in suboptimal efficiency over extended periods of operation. The internal mechanisms involved in the storage of hydrogen in solid-state forms have been extensively investigated due to their exceptional gravimetric and volumetric energy