International Journal of Hydrogen Energy 87 (2024) 966–984

Contents lists available at ScienceDirect

International Journal of Hydrogen Energy

journal homepage: www.elsevier.com/locate/he

Investigation on the hydrogen storage properties, electronic, elastic, and thermodynamic of Zintl Phase Hydrides XGaSiH (X = sr, ca, ba)

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ARTICLE INFO

Handling Editor: Dr M Mahdi Najafpour

Keywords:
Zintl phase hydrides
Hydrogen storage
Elastic constants
Quasi-harmonic debye model

ABSTRACT

This study presents a comprehensive investigation of the electronic, mechanical, and thermodynamic properties of Zintl phase hydrides XGaSiH (X = Sr, Ca, Ba) using Density Functional Theory (DFT) and the FP-LAPW method within the WIEN2k package. Our analysis covers the structural stability, electronic properties, and hydrogen interaction mechanisms in these compounds. The hydrides exhibit narrow band gaps, with values ranging from 0.1 to 0.5 eV using GGA and LDA functionals, and 0.6–1.0 eV with mBJ-GGA and mBJ-LDA. The hydrogen storage capacities are determined to be 0.34 wt %, 0.47 wt %, and 0.40 wt % for SrGaSiH, CaGaSiH, and BaGaSiH, respectively, highlighting their potential for energy storage applications. Thermodynamic properties, evaluated through the quasi-harmonic Debye model, provide insights into the Grüneisen parameter, heat capacity, and thermal expansion coefficient over a range of pressures (0–50 GPa) and temperatures (up to 1000 K). Elastic constants reveal that these compounds are mechanically stable, with a notable anisotropy in the {100} plane and varying degrees of compressibility among the different hydrides. Our study further highlights the slightly ordered hexagonal Ga and Si layers, which contribute to the enhanced hydrogen storage capabilities of these materials. The compounds demonstrate high structural stability, facilitating effective hydrogen retention and release at practical temperatures, making them promising candidates for hydrogen storage applications. Additionally, the analysis of electronic band structures and density of states suggests significant conductivity potential, with band gaps ranging from 0.1 to 1.0 eV, depending on the computational method used. The unique combination of structural, electronic, thermodynamic, and mechanical properties in XGaSiH compounds positions them as valuable materials for renewable energy applications. These findings lay the groundwork for future research focused on optimizing these materials through structural modifications or doping to enhance performance metrics such as hydrogen storage capacity and electrical conductivity.

1. Introduction

In recent years, there has been an increased demand for research in sustainable and renewable energy sources due to growing concerns about the depletion of traditional fossil fuels such as oil, coal, and gasoline [1]. The consumption of these resources has led to harmful environmental impacts, such as greenhouse gas emissions and climate change, prompting the global community to seek cleaner and more sustainable energy alternatives. In this context, hydrogen energy has emerged as a pivotal solution due to its high abundance, energy content, and sustainability [2]. When used as a fuel, hydrogen produces only water as a byproduct, making it an environmentally friendly option.

Parallel to the growing interest in renewable energy, hydrogen storage technologies have become a major focus due to their critical role in advancing the transition to sustainable energy sources. Among these technologies, electrochemical hydrogen storage methods have emerged

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https://doi.org/10.1016/j.ijhydene.2024.09.087
Received 30 July 2024; Received in revised form 5 September 2024; Accepted 6 September 2024