1er Séminaire National :
Eau, Environnement et Energies renouvelables

SN3ER'24

M'Sila, 13 – 14 Octobre 2024

Laboratoire Eau, Environnement et Energies Renouvelables (L3ER)

ATTESTATION DE PARTICIPATION

Le Président du 1er Séminaire National "Eau, Environnement et Energies Renouvelables", organisé par le Laboratoire "Eau, Environnement et Energies renouvelables (L3ER)" et qui s'est tenu les 13 & 14 Octobre 2024 à l'Université de M'sila, atteste que :

Ammi Hadjer

a présenté une **Communication Poster** intitulée : **Investigation on the hydrogen storage properties, electronic of Zintl Phase Hydrides XGaSiH (X = Sr, Ca, Ba)**

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Le Président du Séminaire
Pr. Merzouk Belkacem

Investigation on the hydrogen storage properties, electronic of Zintl Phase Hydrides XGaSiH (X = Sr, Ca, Ba)

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Abstract

This study presents a comprehensive investigation of the electronic and mechanical properties of Zintl hydrides XGaSiH (X = Sr, Ca, Ba) using density functional theory (DFT) and the FP-LAPW method within the WIEN2k package. The analyses include structural stability, electronic properties, and hydrogen interaction mechanisms in these compounds. The hydrides exhibit narrow band gaps ranging from 0.1 to 0.5 electron volts using GGA and LDA functionals, and from 0.6 to 1.0 electron volts using mBJ-GGA and mBJ-LDA functionals. Hydrogen storage capacities were determined to be 0.34%, 0.47%, and 0.40% for SrGaSiH, CaGaSiH, and BaGaSiH, respectively, highlighting their potential for energy storage applications. The elastic constants indicate that these compounds are mechanically stable, with notable anisotropy in the {100} plane and varying degrees of compressibility among different hydrides. The slightly interconnected hexagonal layers of Ga and Si contribute to enhancing the hydrogen storage capabilities of these materials. Electronic structure and density of states analyses reveal significant conductivity potential, with band gaps ranging from 0.1 to 1.0 electron volts depending on the computational method used. The unique combination of structural and electronic properties of XGaSiH compounds positions these materials as promising candidates for renewable energy applications [1].

These results provide a foundation for future research focusing on improving these materials through structural modifications or doping to enhance performance metrics such as hydrogen storage capacity and electrical conductivity. This study offers an in-depth insight into the fundamental properties of Zintl hydrides XGaSiH (X = Sr, Ca, Ba), indicating their significant potential for energy storage applications. With good hydrogen storage capacities and notable structural stability, these materials are particularly promising in the field of renewable energy. The findings enhance the current understanding of how performance can be improved through structural modifications or doping, opening new avenues for research in enhancing storage capacity and electrical conductivity. Future research in improving these materials will significantly contribute to the development of clean and sustainable energy technologies.

Keywords: DFT, Structural properties, Density of states, Zintl hydrides, hydrogen storage.

Reference :

[1] Ammi, H., Charifi, Z., Baaziz, H., Ghellab, T., Bouhdjer, L., Adalla, S., ... & Uğur, G. (2024). Investigation on the hydrogen storage properties, electronic, elastic, and thermodynamic of Zintl Phase Hydrides XGaSiH (X= sr, ca, ba). *International Journal of Hydrogen Energy, 87*, 966-984.