World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:13, No:11, 2019

# Atomic Hydrogen Storage in Hexagonal GdNi5 and GdNi4Cu Rare Earth Compounds: A Comparative Density Functional Theory Study

**Authors :** A. Kellou, L. Rouaiguia, L. Rabahi

**Abstract :** In the present work, the atomic hydrogen absorption trend in the GdNi5 and GdNi4Cu rare earth compounds within the hexagonal CaCu5 type of crystal structure (space group P6/mmm) is investigated. The density functional theory (DFT) combined with the generalized gradient approximation (GGA) is used to study the site preference of atomic hydrogen at 0K. The octahedral and tetrahedral interstitial sites are considered. The formation energies and structural properties are determined in order to evaluate hydrogen effects on the stability of the studied compounds. The energetic diagram of hydrogen storage is established and compared in GdNi5 and GdNi4Cu. The magnetic properties of the selected compounds are determined using spin polarized calculations. The obtained results are discussed with and without hydrogen addition taking into account available theoretical and experimental results.

**Keywords :** density functional theory, hydrogen storage, rare earth compounds, structural and magnetic properties
**Conference Title :** ICACMME 2019 : International Conference on Advances in Chemical, Metallurgical and Materials Engineering
**Conference Location :** Dublin, Ireland
**Conference Dates :** November 07-08, 2019