

## Atomic Hydrogen Storage in Hexagonal GdNi<sub>5</sub> and GdNi<sub>4</sub>Cu Rare Earth Compounds: A Comparative Density Functional Theory Study

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**Abstract :** In the present work, the atomic hydrogen absorption trend in the GdNi<sub>5</sub> and GdNi<sub>4</sub>Cu rare earth compounds within the hexagonal CaCu<sub>5</sub> 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 GdNi<sub>5</sub> and GdNi<sub>4</sub>Cu. 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

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