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HYDROGEN STORAGE IN FUNCTIONALIZED BORAZINE: A DENSITY FUNCTIONAL THEORY APPROACH

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ABSTRACT

Storage of alkali and transition functionalized $B_3N_3H_6$ for hydrogen storage has been studied using Density Functional Theory method. We found that $B_3N_3H_6Li$, $B_3N_3H_6Ti$ can interact with maximum two and five hydrogen molecules respectively with respective gravimetric hydrogen uptake capacity of 4.40 and 7.28 wt % respectively. The uptake capacity has been calculated excluding the weight of hydrogen atoms which are bonded to Boron and Nitrogen. The hydrogen adsorption energies, different structural parameters are obtained for these complexes. The hydrogen adsorption energies obtained are in the range of physisorption and chemisorptions which is essential for a material to be ideal for hydrogen storage.

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