Hydrogen storage materials: A first-principles study

A sustainable provision of energy is one of the greatest challenges to mankind. Energy generated from sustainable sources has to be transported and stored in an efficient and ecologically friendly way. Hydrogen is an important energy carrier in current sustainable energy scenarios. Such scenarios are only realistic, however, if hydrogen can be stored in a light, compact, fast and reliable way, and under moderate conditions. Using materials that absorb hydrogen is one route that can lead to these goals. The present work is devoted to a first-principles study of the hydrogen storage properties of a number of promising bulk, nano and molecular materials.

In the first part, storage materials are considered that store hydrogen in atomic form. The focus is on the bulk properties of magnesium-dihydride (MgH_2) and its alloys with lightweight transition metals (TMs) and aluminum or silicon. We find that TM-alloying initiates a phase transition that results in a significant enhancement of the usually slow (de)hydrogenation kinetics. For the most promising candidates, the Mg-Ti hydrides, we have established that this phase transition occurs both in ordered structures, as well as in random alloy hydrides. Adding aluminum or silicon to Mg-Ti greatly improves the thermodynamic properties by stabilizing the alloys and destabilizing their hydrides, which makes these materials more suitable for practical hydrogen storage applications.

In the second part, materials are considered that store hydrogen in molecular form, which leads to fast kinetics. Metal organic frameworks (MOFs) doped with alkali or alkaline earth metals have been suggested as hydrogen storage media. We find, however, that such doping has a detrimental effect on the structure of a MOF. As an alternative, we studied polylithiated carbon and oxygen molecules as building blocks for hydrogen storage materials and find that these molecules show promising hydrogen storage properties both in the gas and in the condensed phases. Finally, we show that planar boron sheets decorated with alkali metals have very promising hydrogen storage properties.

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