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Materials for Hydrogen Storage: From Nanostructures to Complex Hydrides

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The limited supply of fossil fuels, its adverse effect on the environment, and growing worldwide demand for energy has necessitated the search for new and clean sources of energy. The possibility of using hydrogen to meet this growing energy need has rekindled interest in the study of safe, efficient, and economical storage of hydrogen. This talk will discuss the issues and challenges in storing hydrogen in light complex hydrides and discuss the role of nanostructuring and catalysts that can improve the thermodynamics and kinetics of hydrogen. In particular, we will discuss how studies of clusters can help elucidate the fundamental mechanisms for hydrogen storage and how these can be applied in Boron Nitride and Carbon nanocages and how metallization of these nanostructures is necessary to store hydrogen with large gravimetric density. We will also discuss the properties of complex light metal hydrides such as alanates and magnesium hydrides that can store up to 18 wt % hydrogen, although the temperature where hydrogen desorbs is rather high. Using first principles calculations, we will provide a fundamental understanding of the electronic structure and stability of these systems and how it is affected due to catalysts. It is hoped that the understanding gained here can be useful in designing better catalysts as well as hosts for hydrogen storage.