Computational studies on materials for hydrogen storage

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Hydrogen storage is a critical enabling technology for H2 use as an energy carrier. Achieving safe, efficient and cost-efficient hydrogen storage is essential to our nation if it is to shift to a hydrogen economy. The low volumetric density of gaseous hydrogen requires a storage method that exhibits the highest possible hydrogen packing density. In addition, hydrogen storage media must also be able to rapidly uptake and release hydrogen reversibly near ambient conditions.

There is a renewed interest in the complex hydrides, due in part to the work by Bogdanovic and Schivickardi They demonstrated that NaAlH4 can be used as a reversible hydrogen storage material by the addition of a few percent of selected Ti compounds as catalyst. Although there have been a large number of studies since their pioneering work, the mechanism and the role of such catalysts are still hotly debated.

The goal of our project is to understand the mechanism of reversible hydrogen uptake/release. REU students will perform a series of calculations on different hydrides with varying hydrogen content. The projects will be focused on LiBH4- and LiAlH4-systems. This will provide the students with opportunities to build skills related to computational chemistry and materials science. The students will also develop an appreciation of the importance of computation/modeling in materials development and will be able to apply these skills as these techniques become more prevalent in the future.