Complex hydrides for hydrogen storage – insight through combination of experiment and theory.

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The light complex metal hydrides focus research interest over the last decade as these compounds are considered as a potential storage media for hydrogen. At present the hydrogen release temperatures from these materials are far from optimal; they have complex decomposition paths or problematic reversibility. Some recent research directions aim for synthesis of multi-cation compositions or framework structures; analysis and modification of decomposition paths and intermediate products; detailed, atomic scale, analysis of dynamics and diffusion or establishing reliable methods for metal borohydrides thermodynamic destabilization via eutectic mixing or nano-confinement. The basic properties of the lightest metal borohydride ($LiBH_4$) are still not entirely explained.

Here, the intensive studies of metal borohydrides are strongly supported by theoretical methods that serve as help for interpretation of the experimental data. Recent advances in experimental/theoretical studies of light metal borohydrides will be presented. Theoretical calculations are based on density functional theory. The studies will be illustrated with examples of crystal structure determination, studies of dynamical and transport properties, and calculations of NMR parameters. The later allows elucidation of the properties of nanoconfined systems that pose a challenge for experimental research.