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First-Principles Prediction of Crystal Structures, Reaction Pathways, and Intermediate Products in Hydrogen Storage Reactions[1]

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Practical hydrogen storage for mobile applications requires materials that exhibit high hydrogen densities, low decomposition temperatures, and fast kinetics for absorption and desorption. Unfortunately, no reversible materials are currently known that possess all of these attributes. Here we present an overview of our recent efforts aimed at developing a first-principles computational approach to the discovery of novel hydrogen storage materials. We have developed computational tools which enable accurate prediction of decomposition thermodynamics, crystal structures for unknown hydrides, and thermodynamically preferred decomposition pathways. We present examples that illustrate each of these three capabilities. Specifically, we focus on recent work on crystal structure and dehydriding reactions of (i) borohydride materials, such as $Ca(BH_4)_2$ and $Mg(BH_4)_2$, (ii) amidoboranes and their decomposition products, and (iii) mixtures of complex hydrides.

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