An Investigation of Screening Perovskite-type Hydrides for Hydrogen Storage: First-Principles Study

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Perovskite-type hydrides have great potential to store hydrogen. Using density functional theory (DFT) calculations, the stability and hydrogen release properties have been examined to screen the promising light hydrides for hydrogen storage. All possible perovskite-type hydrides formed by alkali metals (Li, Na, K, Rb, or Cs) and alkaline metals (Be, Mg, Ca, Sr, or Ba) were considered. The most favorable formation and dehydrogenation pathway for each system was obtained. $NaCaH_3$ was found to be the most potential hydride to store hydrogen. The influence of alkali and alkaline-earth dopants of hydrogen release from $NaCaH_3$ was analyzed. The reaction enthalpies of every doping system with different pathways were also calculated. Cs was the most beneficial dopant to improve the hydrogen release due to the lowest reaction enthalpy. However, using alkaline-earth dopants was no clear effects to facilitate the dehydrogenation of $NaCaH_3$. Valuable models can be provided in this study to design new excellent materials for hydrogen storage.