First-Principles Investigation of Light Perovskite-type Hydrides and the Properties of Hydrogen Release

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Light perovskite-type hydrides are one of the promising materials for hydrogen storage due to the high gravimetric hydrogen density. To search for beneficial light hydrides to store hydrogen and explore their properties for hydrogen release, the perovskite-type hydrides ABH3 composed by alkali metals A (A = Li, Na, K, Rb, or Cs) and alkaline metals B (B = Be, Mg, Ca, Sr, or Ba) have been examined using density functional theory (DFT) method. 25 optimized structures including new designed structures and their formation energies are obtained. The hydrogen decomposition energies of all systems are calculated by 3 different pathways. In addition, NaCaH3 is screened to be as one of the most potential material for hydrogen storage. To facilitate the dehydrogenation of NaCaH3, the alkaline dopants (Be, Mg, Sr, or Ba) and alkali dopants (Li, K, Rb, or Cs) are introduced to replace the Ca and Na sites in NaCaH3 structure, respectively. Among them, Cs is the most favorable one to reduce hydrogen desorption energy. These studies will provide valuable model for future experiment and theoretical researches to design excellent hydrides for hydrogen storage.