Hydrogen Desorption Properties of $LiBH_4$ Surface with Dopants: A First-Principles Study

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Due to the high energy density and lightweight, LiBH4 has been viewed as one of the attractive candidates for hydrogen storage. However, more moderate conditions are required for the hydrogen desorption of LiBH4. Hence, the structural stabilities and hydrogen desorption properties of LiBH4 surface with some metals M (M = Na, K, Al, F or Cl) dopants were investigate by the density functional theory (DFT) method. On the basis of all possible surface structures of LiBH4 with different dopants to release hydrogen, the stable structures and formation energies were obtained. Thus, by comparing all the results, the most favorable dopant was found. In addition, the strain effects on the surface of LiBH4 for the hydrogen desorption were calculated. The application of strain has great influence on reducing formation energy for the hydrogen desorption. It means that the dopant and strain played an important role in the hydrogen desorption. These studies present an efficient method to design new promising hydrides with excellent properties for hydrogen storage