The Improvement of Hydrogen Release for $LiBH_4$ (010) Surface Using Strain and Dopants (Na, K, Al, F or Cl)

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Due to the high gravimetric hydrogen density and light weight, the complex metal hydride LiBH4 is a promising candidate for hydrogen storage. The strain (−3% − +3%) and dopants (M = Na, K, Al, F, or Cl) were used to facilitate the dehydrogenation of LiBH4 (010) surface. The structural and chemical effects were investigated by density functional theory (DFT) method. The desorption property can be promoted by weakening the B-H interactions under the tensile strain. Among all dopants examined, Al is the most favorable one to reduce hydrogen desorption energy. The order of dopants for improving hydrogen release is Al > Cl > F > Na > K. However, the Al and Cl co-doping system is the most effective one for tuning hydrogen release with the lowest hydrogen desorption energy. In summary, great influence on improving the dehydrogenation of LiBH4 hydride can be found by the application of tensile strain and dopants. These methods can destabilize metal hydrides to tune the hydrogen release process. Thus, it will be helpful to provide efficient means for improving the hydrogen storage performance of new excellent hydrides.