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First-principles Modeling of Diffusion during Hydrogenation of $LiBH_4$ CHAO YU, VIDVUDS OZOLINS, Department of Materials Science and Engineering, University of California, Los Angeles — $LiBH_4$ has been studied extensively because of its high volumetric and gravimetric hydrogen content. However, experiments show that hydrogen release is very slow at temperatures up to 300 C, which severely limits applications in mobile storage. Using density-functional theory calculations, we systematically study bulk diffusion of defects during solid-state hydrogenation reactions. The defect concentration and concentration gradients are calculated for a variety of defects, including charged vacancies and interstitials. We find that low concentration gradients limit the rate of hydrogen desorption.

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