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First-principles calculations of mass transport in magnesium borohydride CHAO YU, VIDVUDS OZOLINS, Department of Materials Science and Engineering, UCLA — $Mg(BH_4)_2$ is a hydrogen storage material which can decompose to release hydrogen in the following reaction: $Mg(BH_4)_{2(solid)} \rightarrow \frac{1}{6}MgB_{12}H_{12(solid)} + \frac{5}{6}MgH_{2(solid)} + \frac{13}{6}H_{2(gas)} \rightarrow MgH_{2(solid)} + 2B_{(solid)} + 4H_{2(gas)}$. However, experiments show that hydrogen release only occurs at temperatures above 300 °C, which severely limits applications in mobile storage. Using density-functional theory calculations, we systematically study bulk diffusion of defects in the reactant $Mg(BH_4)_2$ and products $MgB_{12}H_{12}$ and MgH_2 during the first step of the solid-state dehydrogenation reaction. The defect concentrations and concentration gradients are calculated for a variety of defects, including charged vacancies and interstitials. We find that neutral $[BH_3]$ vacancies have the highest bulk concentration and concentration gradient in $Mg(BH_4)_2$. The diffusion mechanism of $[BH_3]$ vacancy in $Mg(BH_4)_2$ is studied using the nudged elastic band method. Our results shows that the calculated diffusion barrier for $[BH_3]$ vacancies is $\approx .2$ eV, suggesting that slow mass transport limits the kinetics of hydrogen desorption.

Chao Yu
Department of Materials Science and Engineering, UCLA

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