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Diffusion-limited Kinetic Pathway for Hydrogen Release from $LiNH_2$/LiH BILJANA ROLIH, VIDVUDS OZOLINS, UCLA — From experimental work on decomposition of hydrogen storage materials it has been suggested that bulk diffusion of metal species is the bottleneck for hydrogen release. In this work we study the underlying mechanism for diffusion reactions in the dehydrogenation of $LiNH_2$. Using first-principle, density functional theory methods we have calculated concentration gradients and diffusivities of neutral and charged defects in $LiNH_2$ and Li_2NH phases. The overall activation energy is obtained from these calculations. The calculated activation energies are found to agree well with experimental work on the kinetics of $LiNH_2$ decomposition, suggesting that diffusion of metal species is a possible method for dehydrogenation of Lithium Amide.

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