

Abstract Submitted
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Bulk Diffusion via a “kick-out” method for Lithium in the decomposition reaction $\text{LiAlH}_4/\text{Li}_3\text{AlH}_6$ BILJANA ROLIH, VIDVUDS OZOLINS, UCLA, OZOLINS TEAM — In the pursuit to find a practical system for hydrogen storage, complex metal hydrides have long been considered as viable candidates due to their high hydrogen content. However, some of the challenges faced with these types of systems are poor thermodynamics or kinetics. The underlying mechanisms, and their limiting processes, for the decomposition of these materials need to be understood. From experimental work on the decomposition of hydrogen storage materials, it has been suggested that bulk diffusion of metal species is the bottleneck for hydrogen release. In this work is the dehydrogenation we investigated the system $\text{LiAlH}_4 \rightarrow \text{LiAlH}_6$ with favorable hydrogen release (5.3 wt %), at moderate temperatures. Using first-principles density functional theory we found the defects facilitating mass transport by calculating individual formation energies, highest concentrations, and activation barriers for defect mobility. The mass transport of Lithium is found to be mediated by a “kick-out” mechanism. The results are used to further our understanding of the fundamental mechanism of mass transport and evaluate the possibility of kinetics as the limiting process in this reaction.

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