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First-principles Modeling of Diffusion Reactions in the Hydrogenation of $NaAlH_4$ KYLE MICHEL, VIDVUDS OZOLINS, University of California, Los Angeles — The hydrogenation of $NaAlH_4$ has been studied extensively since it was discovered that doping with Ti greatly increases its reversible hydrogen storage capacity. Experimental studies have suggested that diffusion of metal-containing defects may be the rate-limiting step in this reaction. We present a model to study the diffusion of defects during a solid-state reaction and apply it to this hydrogen storage reaction. The flux of defects in simple, model systems is calculated and from these values the activation energy for these processes is determined. We find that the activation energy for the diffusion of metal defects matches well to the experimental activation energy for the reaction when doped with Ti. The model that is presented can easily be applied to other systems in which a reaction takes place in the solid state.

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