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**Bulk diffusion of defects in LiAlH<sub>4</sub>/Li<sub>3</sub>AlH<sub>6</sub>** BILJANA ROLIH, VIDVUDS OZOLINS, UCLA — From various experimental studies on decomposition of hydrogen storage materials it has been proposed that bulk diffusion of metal species may be the rate limiting step in hydrogen storage reactions. A recently developed theoretical model uses density functional theory to study the underlying processes involved in bulk diffusion. To date this model has been applied to study dehydrogenation of NaAlH<sub>4</sub>. However further study of alkaline and alkali earth metals merits attention, particularly LiAlH<sub>4</sub> with a high gravimetric hydrogen density, accessible at moderate temperatures. This study uses density functional theory to obtain concentration gradients and diffusivities of native charged and neutral defects in Li<sub>3</sub>AlH<sub>6</sub> and LiAlH<sub>4</sub>. The flux of each defect is obtained and thus the activation energy for each defect. Our results show that diffusion of metal species is a possible rate limiting process in the system.

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