Bulk diffusion of defects in LiAlH4/Li3AlH6 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 NaAlH4. However further study of alkaline and alkali earth metals merits attention, particularly LiAlH4 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 Li3AlH6 and LiAlH4. 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.