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Discovering the Optimal Route for Alane Synthesis on Ti doped Al Surfaces Using Density Functional Theory Based Kinetic Monte Carlo Methods[1] ALTAF KARIM, Center for Functional Nanomaterials, Brookhaven National Lab, JAMES T. MUCKERMAN, Center for Functional Nanomaterials, Department of Chemistry, Brookhaven National Lab — Issues such as catalytic dissociation of hydrogen and the mobility of alane species on Ti-doped Al surfaces are major challenges in the synthesis of aluminum hydride. Our recently developed modeling framework (DFT-based KMC simulation) enabled us to study the steady-state conditions of dissociative adsorption of hydrogen, its diffusion, and its reaction with Al adatoms leading to the formation of alane species on Ti-doped Al surfaces. Our studies show that the doping of Ti atoms in the top layer of Al surfaces significantly reduces the mobility of alane species. On the other hand, the doping of Ti atoms beneath the top layer of Al surfaces enhances the mobility of alane species. The arrangement of dopant Ti atoms in different layers not only affects the diffusion barriers of alane species but it also affects hydrogen dissociation barriers when Ti-Ti pairs are arranged in different ways in the top layer. Using our theoretical methods, we identified a few configurations of dopant Ti atoms having lower barriers for alane diffusion and hydrogen dissociation. Further, we discovered the optimal values of Ti concentration, temperature, and pressure under which the rate of alane formation is maximized.

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