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Density Functional Theory Based Kinetic Monte Carlo Approach for Understanding Atomistic Mechanisms for Reversible Hydrogen Storage in Metal Hydrides: Application to Alane Formation on Ti Doped Al Surfaces[1] A. KARIM, J. MUCKERMAN, P. SUTTER, E. MULLER, BNL — We describe a density functional kinetic Monte Carlo approach enabling us to study and simulate the steady-state situation of dissociative adsorption of hydrogen along with diffusion and reaction of Al and H atoms leading towards the formation of alane species on Ti-doped Al surfaces. In the first step, density functional theory is used in conjunction with the nudged elastic band/drag method to obtain the energetics of the relevant atomistic processes of Al and H diffusion and their reactions on Al surfaces with different concentration of dopant Ti atoms. Subsequently, the kinetic Monte Carlo method is employed, which accounts for the spatial distribution, fluctuations, and evolution of chemical species at Ti-doped Al surfaces under steady-state conditions. This DFT-based KMC approach provides an insight into the kinetics of alanes at technologically relevant pressure and temperature conditions. Our computed production rates of AlH_3 on Al surfaces are in agreement with experimental data. We also obtained temperature programmed desorption spectra of different alane species, which is agreeing well with experiments.

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