DFT and DFT-MD Study of Pure and Doped-$NaMgH_3$ (001) Surface

Authors: Fernando Soto[1], Daniela S. Mainardi[2]

[1]Institute for Micro-manufacturing, Louisiana Tech University, [2]Institute for Micro-manufacturing, Chemical Engineering, Louisiana Tech University

Abstract

Transition-metals (TMs) such as Ti are commonly used in hydrogen-storage materials to increase hydrogen absorption and desorption kinetics. The role of 3d transition metals such as Ti in the improved hydrogen desorption process in $NaMgH_3$ surface needs to be understood in order to overcome one of the main roadblocks currently existing for implementation of hydrogen storage technologies. Using density functional theory (DFT) calculations, we study the effect of 3d transition metals on H-desorption from $NaMgH_3$ (001) surface. Activation energy barriers of the different reaction pathways of hydrogen desorption are calculated via transition-state theory (TST) methods. In addition, DFT is used to determine equilibrium position of relevant species on the surface of $NaMgH_3$. We find that 3d-dopants are effective in reducing kinetic barriers, in agreement with experimental observations for similar materials. Finally, DFT coupled with molecular dynamics is used evaluate the effect of transition metals at high temperatures on hydrogen desorption from $NaMgH_3$ surface. These findings can be used for future design and fabrication of nano-structured hydrogen storage materials.