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**Thermodynamics, kinetics, and catalytic effect of dehydrogenation from MgH2 stepped surfaces and nanocluster: a DFT study** JASON REICH, Department of Chemistry, University of Illinois at Urbana Champaign, LIN-LIN WANG, Ames Laboratory, U.S. Department of Energy, DUANE JOHNSON, Ames Laboratory, U.S. Department of Energy; Department of Materials Science & Engineering, Iowa State University — We detail the results of a Density Functional Theory (DFT) based study of hydrogen desorption, including thermodynamics and kinetics with(out) catalytic dopants, on stepped (110) rutile and nanocluster $MgH_2$. We investigate competing configurations (optimal surface and nanoparticle configurations) using simulated annealing with additional converged results at 0 K, necessary for finding the low-energy, doped $MgH_2$ nanostructures. Thermodynamics of hydrogen desorption from unique dopant sites will be shown, as well as activation energies using the Nudged Elastic Band algorithm. To compare to experiment, both stepped structures and nanoclusters are required to understanding and predict the effects of ball milling. We demonstrate how these model systems relate to the intermediary sized structures typically seen in ball milling experiments.

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