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Thermodynamic and kinetic size effects for hydrogen-desorption in catalytically-doped magnesium hydride: Nanoparticle versus bulk surface effects[1] JASON REICH, Chemistry, L.-L. WANG, D. D. JOHNSON, Materials Science and Engineering — Using density-functional methods with simulated annealing, we show that there are no size effects for hydrogen desorption energies in nanoparticles (NPs) of MgH2. Recently reported exothermic desorption energies in MgH2-doped NP (Mg30XH62) are shown to be spurious, resulting from metastable NP configurations before dehyrogenation. We confirm that the 93-atom NPs are amorphous, with structures that are sensitive to the presence of dopants, found via simulated annealing techniques. We find that dehydrogenation energies are similar between bulk surfaces and nanoparticles, showing that the thermodynamics is unchanged by particle size as desorption is determined only by the local hydrogen-metal bond. We then discuss the effects of nanoparticle size and presence of dopants on the kinetic barriers between NPs and bulk surfaces. The takehome message is: In modeling desorption events, especially within amorphous NPs, metastable, local minimum must be carefully avoided, and, in doing so, an accurate and physically reasonable picture emerges for the thermodynamic and kinetic behavior.

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