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Title: Critical Roles of Nanostructures in Hydrogen Storage

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Onboard hydrogen storage requires a hydrogen binding energy that does not exist in naturally occurring materials. Either the binding energy is too high, as with hydrides, or too low, as with gas sorbents. Recently, we suggested that hydrogen binding energy to gas sorbents can be significantly enhanced [1-3]. The key is to find a way to disperse undercoordinated metal atoms on lightweight carbon nanostructures. Here, we take another approach and examine hydrogen desorption from metal hydrides with and without the catalyst. We consider the catalyzed hydrogen desorption process to be a global process involving hydrogen release, transport, and H2 liftoff, rather than a local process involving only the reduction in the H2 liftoff barrier by the catalyst at the surfaces. In particular, we will discuss Pd catalyzed dehydrogenation of MgH2. For this simple binary compound, our first-principles calculations reveal two global dehydrogenation pathways that are enabled by the Pd. One of the pathways has a noticeably smaller overall hydrogen desorption barrier and the process is self-terminating when the material approaches bulk. The results agree with experiments. Our findings thus clarify the critical role of nanostructures in catalyzing hydrogen desorption from metal hydrides. This ongoing study, combined with earlier work on hydrogen sorbents, unifies the critical roles of nanostructures in hydrogen storage. [1] Y. Zhao, et al., Phys. Rev. Lett. 94, 155504 (2005). [2] Y.-H. Kim, et al., Phys. Rev. Lett. 96, 016102 (2006). [3] L Wang, et al., ACS Nano 3, 2995 (2009).