

Abstract Submitted
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Effect of transition-metal additives on dehydrogenation kinetics of MgH_2 ¹ ANINDYA ROY, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California Santa Barbara — Using first-principles calculations based on hybrid density functional theory we study the (de)hydrogenation process in MgH_2 , an important solid-state hydrogen storage material. This reaction proceeds through diffusion processes, mediated by native point defects such as vacancies and interstitials. Reducing the formation energy of relevant defects increases their concentrations, resulting in higher diffusion rates and an enhancement in kinetics. We investigate the formation energies of native point defects in MgH_2 and determine the position of the Fermi level in the band gap using the charge neutrality condition. The presence of transition-metal (TM) impurities (Ti, Fe, Co and Ni) causes the Fermi level to shift according to the position of the TM acceptor/donor levels in the band gap. This shift can bring down the formation energy of native defects. Our calculations predict that all of the TM additives, in either interstitial or substitutional configurations, may cause such a shift in the Fermi level and thus increase the concentration of the hydrogen vacancies that govern hydrogen diffusion. Our proposed mechanism explains the experimentally observed enhancement in the rate of dehydrogenation of MgH_2 upon addition of TM impurities.

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