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Role of nano in catalysis: Pd catalyzed H desorption from MgH_2

WEIYU XIE, DAMIEN WEST, YIYANG SUN, SHENGBAI ZHANG, Rensselaer Polytech Inst — Magnesium hydride (MgH_2) is promising for on-board hydrogen (H) storage with the major hurdle being the slow desorption kinetics. H desorption from ball-milled MgH_2 peaks at two slightly different temperatures, which further split in the presence of palladium catalyst. It has been experimentally demonstrated that nanostructuring can eliminate the high temperature peak. However, the effect of nanostructuring cannot be explained by thermodynamic destabilization due to quantum size effect. Our first-principles calculation reveals that there exist two reaction pathways for H desorption from MgH_2. One involves H vacancy (SV) diffusion at surface, while the other one involves H atom diffusion in bulk. The SV pathway self-terminates as dehydrogenation eventually eliminates the exposed MgH_2 region. Therefore, it is size-sensitive and fully functions only when the surface-to-bulk ratio is large, which is available only in nanostructures. Our calculation further shows that the SV pathway significantly lowers the desorption barrier, because it decouples the H transport process with the surface liftoff process and benefits from a fact that diffusion of vacancies at surface can have significantly lower barrier than that in bulk.

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