

Abstract Submitted
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Hydrogen desorption from MgH₂(110) surface with transition-metal catalyst: a DFT study of energetics and barriers¹ LIN-LIN WANG, DUANE D. JOHNSON, Division of Materials Science and Engineering, Ames Laboratory/US DoE, Iowa State University, Ames, IA 50011-3020 — Transition-metal (TM) catalysts are widely used in hydrogen-storage materials to increase hydrogen absorption and desorption kinetics. Using density functional theory calculations, we elucidate the catalytic effect of Ti on H-desorption from MgH₂(110) surface. Kinetic energy barriers of different reaction pathways of hydrogen desorption are calculated via nudged-elastic-band method. We find that Ti dopant is effective in reducing kinetic barriers, in agreement with experimental observations. We also find that magnetic degrees of freedom must be carefully included to describe the change of magnetic states during catalytic-enhanced desorption. As vacancy migration barriers are lower than desorption barrier, bulk diffusion of H inherently feeds into the favorable surface desorption mechanism.

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