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Understanding and Enhancing Hydrogen Diffusion in MgH_2 and $NaMgH_3$ DAVID SHOLL, SHIQIANG HAO, Georgia Tech — The transport properties of hydrogen in metal hydrides are crucial to the kinetics of H_2 storage in these materials. We use first-principles calculations to identify the defects that are relevant for H transport in MgH_2 and $NaMgH_3$. In both materials, the physically relevant defects are charged and H diffusion is dominated by mobility of negatively charged interstitial H. Interestingly, the diffusion of these species occurs via concerted mechanisms with low energy barriers. To improve the charged interstitial H diffusivity, a series of transition-metal additives are screened to lower the formation energy of mobile defects. Our results provide a practical way to examine and alter H diffusion in light metal hydrides.

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