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Pressure-induced hydrogen storage mechanisms of TM-doped MgH2

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Hydrogen storage technology has attracted a worldwide interest for enhancing the efficiency of hydrogen energy carrier used in a clean energy innovation mobile car. In this work, ab initio study of hydrogen storage mechanisms in Magnesium hydride (MgH2) with doping transition metals (TM) was analyzed. High-pressure and structural effects on the doped MgH2 were examined. The conventional cells were optimized and calculated the physical properties using Kohn-Sham equations with GGA-PBE functional. Enthalpy of formation and the potential barrier of kinetics hydrogen diffusion were analyzed under pressure increasing. It was found that Ni and Pd reduces enthalpy of formation and the potential barrier of kinetics hydrogen diffusion in the doped MgH2.

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