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Lowering the desorption temperature of $Mg(BH_4)_2$ through doping[1] D. HARRISON, T. THONHAUSER, Wake Forest University — Magnesium borohydride $Mg(BH_4)_2$ is a very promising hydrogen storage material due to its high gravimetric (14.9 mass%) and volumetric density. However, it is limited for practical storage applications by its high hydrogen desorption temperature of 270°C. Arguments have been made for both high thermodynamic stability and slow kinetics to be responsible for this high desorption temperature. In our study we show that doping of $Mg(BH_4)_2$ can address the thermodynamic stability issue and predictably lower its desorption enthalpy. We use ab initio calculations at the DFT level (utilizing vdW-DF) and calculate the change in desorption enthalpy from ground state energy and phonon contributions for several possible hydrogen release reactions. Note that van der Waals interactions are crucial to correctly describe the ground state of this complex hydride. We find that, depending on the reaction, the undoped phase has a desorption enthalpy of 50–75 kJ/mol H_2 and doping can lower this number by approximately 5 kJ/mol per 10% doping at 300 K, making the desired range of 40 kJ/mol easily accessible. We argue that this lowering of desorption enthalpy will correspond to a lowering of the desorption temperature.

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