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TiH2 for improving the rehydrogenation properties of MgH2

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Abstract
The present study reports the results of an experimental and theoretical study of de/rehydrogenation in the MgH2-TiH2. The experimental study shows that TiH2 improves the thermodynamics and kinetics of de/rehydrogenation in Mg/MgH2. It has been observed that the MgH2-TiH2 absorbs 4.00 and 0.60 wt.% more hydrogen as compared to ball milled MgH2 and MgH2-Ti system respectively. The reaction enthalpy for ball milled MgH2 and MgH2-Ti system remains unchanged but the enthalpy change for MgH2-TiH2 system is nearly ~7kJ/mol lower. On the basis of XRD,TEM studies suitable crystallographic model for theoretical calculations has been developed. The theoretical models are being further explored to understand the reason for lowering of reaction enthalpy in Mg/MgH2-TiH2. The Interface energy calculations (DFT) well supported by micro structural study are being done to find the preferred location of TiH2 in Mg/MgH2-TiH2 system. The feasible mechanism for working of TiH2 as additive in MgH2-TiH2 is being worked out.
Keywords: Energy, DFT, MgH2