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Energetics of Hydrogen Storage Reactions: The Power of DFT

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Calculations of hydrogen site energetics in LaNi_5H_n (hexagonal $\text{P6}_3\text{mc}$ crystal structure) and LaCo_5H_n (orthorhombic Cmmm structure) have been performed within density functional theory (DFT). In each case DFT correctly identifies the most stable hydrogen site configuration, yields an accurate value for the enthalpy of hydride formation, and predicts hydrogen-richer hydrides. The novel hydrogen storage reaction $\text{LiNH}_2 + \text{LiH} \leftrightarrow \text{Li}_2\text{NH} + \text{H}_2$ has also been investigated, with the inclusion of zero point energies and finite temperature corrections. The generalized gradient approximation for the exchange-correlation energy functional μ_{xc} provides much better agreement with experiment than the local density approximation for the structural parameters as well as for the enthalpy of formation of LiNH_2 , LiH , and the reaction enthalpy. While the choice of μ_{xc} may have substantial impact on results, it is indisputably clear that DFT is a powerful tool for understanding hydrogen storage energetics.