

Abstract Submitted
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Hydrogen-related defects and the role of metal additives in complex hydrides¹ KHANG HOANG, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Complex hydrides such as NaAlH_4 and $\text{Li}_4\text{BN}_3\text{H}_{10}$ doped with selected transition metals (e.g., Ti, Ni, and Pt) are promising hydrogen storage materials. The mechanism of the enhancement in (de)hydrogenation rates caused by these metals is, however, not well understood. We have carried out first-principles studies based on density functional theory of hydrogen vacancies and interstitials, which play an important role in the (de)hydrogenation processes. We find that these defects are always charged; their formation energy therefore depends on the Fermi level. The metallic impurities can also exist in different charged states and, therefore, modify the Fermi level, thus changing the defect concentrations. Our first-principles results shed light on the role of transition-metal impurities in hydrides and lead to the design of storage materials with improved characteristics.

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