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Hydrogen-related defects and the role of Ti in NaAlH4[1] AMRA PELES, CHRIS VAN DE WALLE, University of California Santa Barbara — Titanium-doped sodium alanate is a promising storage material; however, the mechanism of the enhancement in (de)hydrogenation rates induced by Ti has remained unresolved. We performed a comprehensive investigation of hydrogen vacancies and interstitials, which play an important role in the (de)hydrogenation processes. Interestingly, these highly mobile defects cause large rearrangements of the surrounding lattice, and they are always charged; their formation energy therefore depends on the Fermi level. Our investigations show that the Ti-induced modification of the Fermi level increases the defect concentrations, thus explaining the improved kinetics. These novel insights may prompt a reexamination of the role of transition-metal impurities in alanates and related materials, and lead to the design of storage materials with improved characteristics.

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