

Abstract Submitted
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LiNH₂–MgH₂ as a Potential Hydrogen Storage Material: a Density Functional Theory Study RALPH H. SCHEICHER, C. MOYSES ARAUJO, Uppsala University, Sweden, RAJEEV AHUJA, Uppsala University, Sweden; KTH, Stockholm, Sweden — LiNH₂ possesses high capacity for hydrogen storage [1], but its large hydride formation enthalpy leads to operating temperatures and pressures that lie outside the practicable range for vehicular applications. Partial substitution of Li by Mg can destabilize the system and thus improve the hydrogen de-sorption characteristics, as it has been shown in recent experimental studies [2]. We present and discuss results from our density functional theory investigations of the LiNH₂–MgH₂ system. The main aim of this study is to understand the bonding characteristics, the Mg-induced destabilization mechanism, and the thermodynamics of hydrogen de-sorption from an electronic structure viewpoint. [1] P. Chen et al., J. Phys. Chem. B 107, 10967 (2003). [2] W. Luo, J. Alloys Compd. 381, 284 (2004).

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