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More insights into $LiNH_2$-(LiH, MgH_2) system from DFT studies C. MOYSÉS ARAÚJO, RALPH H. SCHEICHER, Condensed Matter Theory Group, Dept of Physics, Uppsala University, Sweden, PURU JENA, Physics Dept, Virginia Commonwealth University, Richmond VA, RAJEEV AHUJA, CMT Group, Uppsala; Applied Materials Physics, Dept of Materials Science and Engineering, Royal Institute of Technology, Stockholm, Sweden — First-principles calculations based on density functional theory have been carried out by us to understand the hydrogen desorption reactions for systems involving $LiNH_2$ mixed with either LiH or MgH_2. We first determined the crystalline structures and total energies of the reactants and possible products, which have been proposed from experiment. Our results for $LiNH_2$ and Li_2NH show good agreement with experimental data. For the mixed compound $Li_2Mg(NH)_2$, we have performed geometry optimization by force minimization and in addition also using molecular dynamics and simulated annealing. The circumstance that the crystalline structure of this system has not yet been resolved prevented us from comparing our results with experimental data. However, the calculated reaction enthalpy agrees very well with recent measurements [1]. Furthermore, we have also investigated all involved reactions in the gas phase by carrying out molecular calculations. This approach has allowed us to achieve a better understanding of the reaction mechanisms. We found that reaction energies for the molecular systems follow the same trend as for the bulk systems. [1] Weifang Luo, J. Alloys Comp. 381, 284 (2004).

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