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Ab-initio Investigations of Li and Mg Amide-Imide Systems for Hydrogen Storage TAKAO TSUMURAYA, TATSUYA SHISHIDOU, TAMIO OGUCHI, Hiroshima University — Reversible hydrogen storage in light-element materials has been recognized as one of the most practical approaches for on-board application. Lithium nitride Li_3N can reversibly store large amount of hydrogen in the two-step reversible reaction composed of lithium amide $LiNH_2$ and imide Li_2NH[1]. Quite recently, in an effort to reach further performance, several types of magnesium substitutions in Li-N-H system have been investigated. For instance, Leng *et al*. have examined a composite material made by ball milling of 3:8 molar mixture of magnesium amide $Mg(NH_2)_2$ and lithium hydride LiH[2]. The hydrogenating and dehydrogenating reaction mechanism and fundamental properties of these hydrides still remain as a matter to be investigated. In particular, crystal structures of some metel imides such as Li_2NH, MgNH and $Li_2Mg(NH)_2$ are not fully determined yet. In this paper, we discuss structural stability and heats of formation of these hydrides from first-principles calculations based on the all-electron FLAPW method. [1] P. Chen Z. Xiong, J. Luo, J. Lin and K.L. Tan, Nature 420, 302 (2002). [2] H. Y. Leng, T. Ichikawa, S. Hino, N. Hanada, S. Isobe and H. Fujii, J. Phys. Chem. B 108, 8763 (2004).

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