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**First-principles Study on Li-N-H System for Hydrogen Storage**
TAKAO TSUMURAYA, TATSUYA SHISHIDOU, TAMIO OGUCHI, ADSM, Hiroshima University — Lithium amide ($LiNH_2$) and lithium imide ($Li_2NH$) have been noticed as one of the most promising candidates for hydrogen storage due to their high gravimetric densities of hydrogen. As regards the hydrogenating and dehydrogenating processes that involve these lithium hydrides, there is an argument about whether ammonia gas is relevant and it still remains as a matter to be studied. Furthermore, the crystal structure of $Li_2NH$ is not fully determined yet because of the difficulty in identifying hydrogen positions. Recently, various transition-metal compounds have been examined with ball milling technique for exploring catalysis to promote reaction processes, and they found that some of the Ti compounds show good performance. Measurements of x-ray absorption spectroscopy (XAS) at Ti K edge are currently under way to have a clue for understanding the catalysis mechanism. To address these issues and to get fundamental insights from microscopic level, we performed first-principles calculations by using all-electron full-potential linear augmented plane wave (FLAPW) method. We will discuss structural stability, electronic structure of lithium hydrides $LiNH_2$ and $Li_2NH$ and the heat of formation in reaction processes. Structural optimization is carried out to evaluate total energies involved in reaction processes. XAS spectra and electronic structure of Ti compounds are also discussed.

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