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First-principles Study on the Vibration Modes and Electronic Structure of Alkali and Alkaline-earth Amides and Alanates TAKAO TSUMURAYA, TATSUYA SHISHIDOU, TAMIO OGUCHI, Hiroshima University — Light alkaline and alkaline-earth metal hydrides such as amides $M(NH_2)_n$ and alanates $M(AlH_4)_n$ (M=K, Na, Li, Ca, and Mg) have attracted a growing interest as reversible hydrogen storage materials recently because of their innately high hydrogen contents. [1, 2] We study the electronic structure of the amides and alanates with different cations, focusing on the role of cation states from first-principles calculations based on the all-electron FLAPW method. Calculated breathing stretch vibration modes for these compounds are compared with measured infrared and Raman spectra. In the amides, we find a significant tendency such that the breathing stretch vibration frequencies and the structural parameters of NH_2 vary in accordance with the ionization energy of cation, which may be explained by the strength in hybridization between cation orbitals and molecular orbitals of $(NH_2)^-$. We elucidate the microscopic mechanism of correlations between the breathing stretch vibration frequencies of N-H and structural parameters by analyzing the calculated electronic structure from a view point of the molecular-orbitals. A similar tendency in the alanates is also discussed. [1] P. Chen, Z. Xiong, J. Luo, J. Lin and K.L. Tan, Nature **420**, 302 (2002). [2] B. Bogdanovi and M. Schwickardi, J. Alloys Compd. **253-254**, 1 (1997).

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