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First-principles investigation of the Li-Mg-N-H system ZHU MA, YAN WANG, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology — The Li-Mg-N-H system has been identified as a promising hydrogen storage material due to its moderate operation conditions as well as the high capacity and reversibility. The Li-Mg mixed imide is reported to have disordered cation or cation-vacancy arrangements at room temperature and above. We present our first-principles investigation to study the crystal structure of $Li_2Mg(NH)_2$ using total energy calculations within the density functional theory. A series of ordered low-energy configurations are identified. Specific local orderings are found in the cation-vacancy arrangement, shedding light on the experimental disordered structure models. A possible ordered phase at lower temperature is proposed based on our calculation. Furthermore, the reaction energetics and phase stability involved in this system are discussed.

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