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First-Principles Study of the Li-Mg-N-H System: Compound Structures and Hydrogen Storage Properties KYLE MICHEL, VIDVUDS OZOLINS, Department of Materials Science and Engineering, University of California, Los Angeles — The Li-Mg-N-H system is studied with the addition of the Li4Mg(NH)3, MgNH, and Li4NH compounds using first-principles density-functional theory (DFT) calculations. A structure for the mixed imide Li4Mg(NH)3 is proposed, belonging to the Imm2 space group. A new structure for Li2Mg(NH)2 is given that has Pca21 symmetry; this compound has been previously reported as having Iba2 symmetry. The stability of the Li4Mg-imide is studied with respect to its decomposition reactions. The static, zero-point (ZPE), and vibrational energies of all relevant compounds belonging to this system are reported along with their predicted lowest-energy structures. Dehydrogenation reactions are presented that involve these phases and which are found to be spontaneously occurring within 400 K of room temperature. It is predicted that mixing LiH, LiNH2, and Li2Mg(NH)2 at 505 K will form Li4Mg(NH)3 with the release of 2.04 wt. % H2.

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