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First-principles study of structural properties of Li_2NH AMRA PELES, Georgia Institute of Technology, Atlanta, Georgia, USA, SUCHISMITA SANYAL, MAHESH CHANDRAN, GE Global Research, John F Welch Technology Centre, Bangalore, 560066 INDIA, JOB RIJSSENBEEK, GE Global Research, 1 Research Circle, Niskayuna, New York, 12309 USA, MEI-YIN CHOU, Georgia Institute of Technology, Atlanta, Georgia, USA — Nitrogen containing hydrides have attracted much attention recently as viable candidates for hydrogen storage materials. One example is the amide and imide involved in the reversible chemical reaction

$$LiNH_2 + LiH \rightarrow Li_2NH + H_2.$$

In an effort to understand the reaction mechanism, one needs to have the informations on the structural properties of these compounds. There is a disagreement in the existing literature regarding the crystal symmetry of Li_2NH. We present a summary of first-principles investigations of the structural properties of Li_2NH in an attempt to identify the lowest energy structure. Calculations were performed within density functional theory framework employing plane waves and projector-augmented-wave potentials. Various crystal structures were obtained by minimazing the total energy and the forces. The stability and energetics of these structures will be discussed.

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