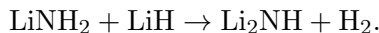


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First-principles study of structural properties of Li₂NH AMRA

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



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 Li₂NH. We present a summary of first-principles investigations of the structural properties of Li₂NH 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 minimizing the total energy and the forces. The stability and energetics of these structures will be discussed.

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