

Abstract Submitted  
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**Role of native defects in the Li amide/Li imide hydrogen storage reaction**<sup>1</sup> KHANG HOANG, CHRIS G. VAN DE WALLE, University of California - Santa Barbara — Reversible reaction involving Li amide/Li imide ( $\text{LiNH}_2 + \text{LiH} \leftrightarrow \text{Li}_2\text{NH} + \text{H}_2$ ) has been shown to be a potential mechanism for hydrogen storage [1]. Recent synchrotron x-ray diffraction refinement suggests that the transformation between  $\text{LiNH}_2$  and  $\text{Li}_2\text{NH}$  is a bulk reaction that occurs through non-stoichiometric processes [2]. To build a deeper understanding of these processes, we have carried out first-principles studies based on density functional theory of native point defects and defect complexes in  $\text{LiNH}_2$  and  $\text{Li}_2\text{NH}$ . Among the native defects, we find that positively and negatively charged Li and H interstitials and vacancies have the lowest formation energies. Some of the Li-related defects are found to be very mobile, and should be the dominant migratory species in the systems. Our first-principles results suggest specific mechanisms for the role of native defects in the Li amide/Li imide reaction. [1] P. Chen *et al.*, *Nature* **420**, 302 (2002). [2] W. I. F. David *et al.*, *J. Am. Chem. Soc.* **129**, 1594 (2007).

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