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**Theoretical Investigation of the Li amide/Li imide Hydrogen Storage Reaction** JAN HERBST, LOUIS HECTOR, JR., GM R&D Center — Considerable recent interest has centered on the reaction $LiNH_2$ + LiH $\leftrightarrow$ $Li_2NH$ + $H_2$ as a mechanism for hydrogen storage. We have conducted density functional calculations of the electronic structure, vibrational properties, and enthalpy of formation for each component. The long established crystal structures for LiH and $LiNH_2$ (Li amide) were employed, while a newly determined orthorhombic structure for $Li_2NH$ (Li imide) was used. Our 298K results within the generalized gradient approximation for $\Delta H(LiNH_2)$ and $\Delta H(LiH)$, as well as for the overall heat of reaction, are in excellent accord with experiment, suggesting that the measured $\Delta H(Li_2NH)$ is inaccurate. Phonon densities of states calculated for the amide and imide compare very favorably with observed infrared and Raman spectra.

Jan Herbst
GM R&D Center

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