Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Theoretical investigation of intermediate phases between Li_2NH and $LiNH_2$ FENG ZHANG, School of Physics, Georgia Tech, YAN WANG, MEI-YIN CHOU — The cycling between Li imide (Li_2NH) and Li amide ($LiNH_2$) represents the key reactions in the Li-N-H hydrogen storage system. It is important to know whether there exist intermediate phases between these two stable compounds in order to fully understand the mechanism of these reactions. We investigate from first principles possible intermediate compounds $Li_{2-x}NH_{1+x}$ and $Li_{1+x}NH_{2-x}$ with x equal to 1/8 and 1/4. $Li_{2-x}NH_{1+x}$ is created by replacing a certain amount of NH^{2-} with NH_2^- in pure Li imide and removing a proper amount of Li^+ to satisfy charge neutrality. Similarly, $Li_{1+x}NH_{2-x}$ is created by replacing a certain amount of NH_2^- with NH^{2-} in Li amide and adding a suitable amount of Li^+. At $T = 0$ K, $Li_{2-x}NH_{1+x}$ is energetically favorable with respect to phase separation into pure Li_2NH and $LiNH_2$. On the amide side, $Li_{1+x}NH_{2-x}$ is only slightly less stable than the phase-separated mixture of amide and imide. These findings suggest that the intermediate phases may appear during the cycling reactions at finite temperatures. Electronic signatures for the intermediate phases resulting from the coexistence of NH_2^- and NH^{2-} anions will also be discussed.

Feng Zhang
School of Physics, Georgia Tech

Date submitted: 20 Nov 2009 Electronic form version 1.4