

# Supporting Information

## An Investigation into the Hydrogen Storage Characteristics of $\text{Ca}(\text{BH}_4)_2:\text{LiNH}_2$ and $\text{Ca}(\text{BH}_4)_2:\text{NaNH}_2$ : Evidence of Intramolecular Destabilization

Natchapol Poonyayant,<sup>1,2</sup> Vitalie Stavila,<sup>2,\*</sup> Eric H. Majzoub,<sup>3</sup> Leonard E. Klebanoff,<sup>2</sup> Richard Behrens,<sup>2</sup> Natee Angboonpong<sup>1,2</sup> Mutlu Ulutagay-Kartin,<sup>2</sup> Pasit Pakawatpanurut,<sup>1</sup> Ethan Hecht,<sup>2</sup> Joe S. Breit<sup>4</sup>

<sup>1</sup> Department of Chemistry, Center for Alternative Energy, and Center of Excellence for Innovation in Chemistry, Faculty of Science, Mahidol University, Bangkok, Thailand

<sup>2</sup> Sandia National Laboratories, Livermore, CA 94551

<sup>3</sup> Center for Nanoscience, Departments of Physics and Astronomy, and Department of Chemistry and Biochemistry, University of Missouri, St. Louis

<sup>4</sup> System Concept Center, Boeing Commercial Airplanes, Everett, WA 98203

\* Corresponding author: : Tel. (925) 294-3059; E-mail: [vnstavi@sandia.gov](mailto:vnstavi@sandia.gov)

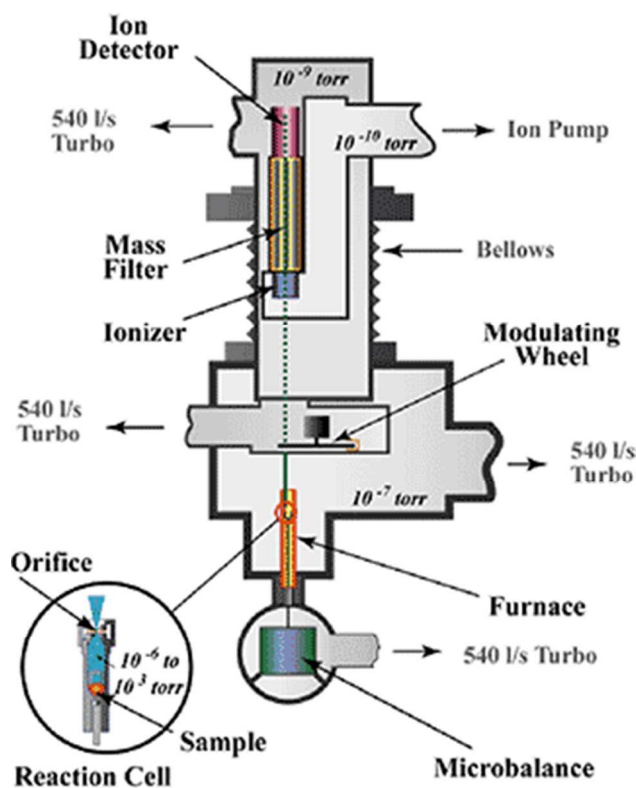
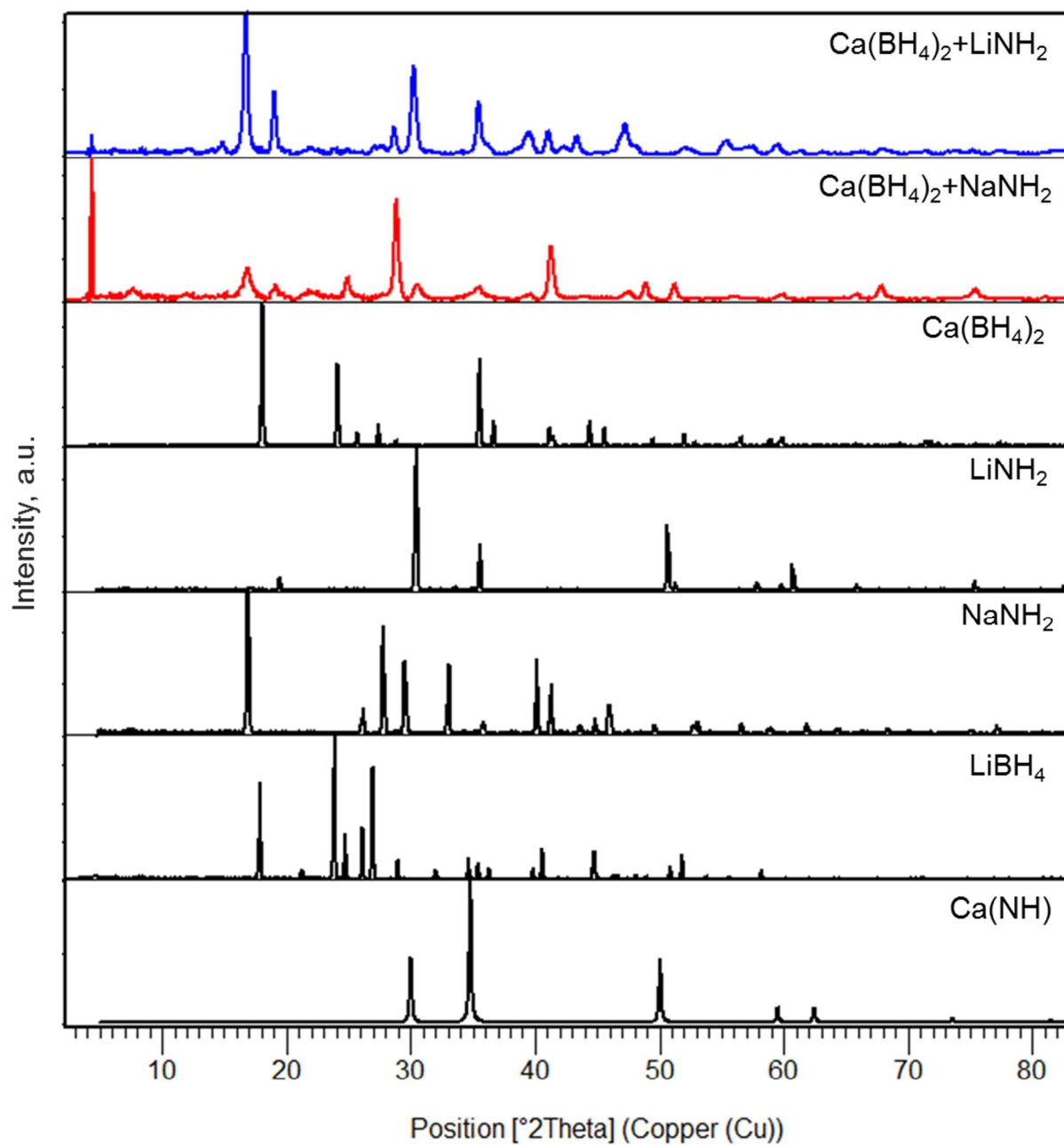
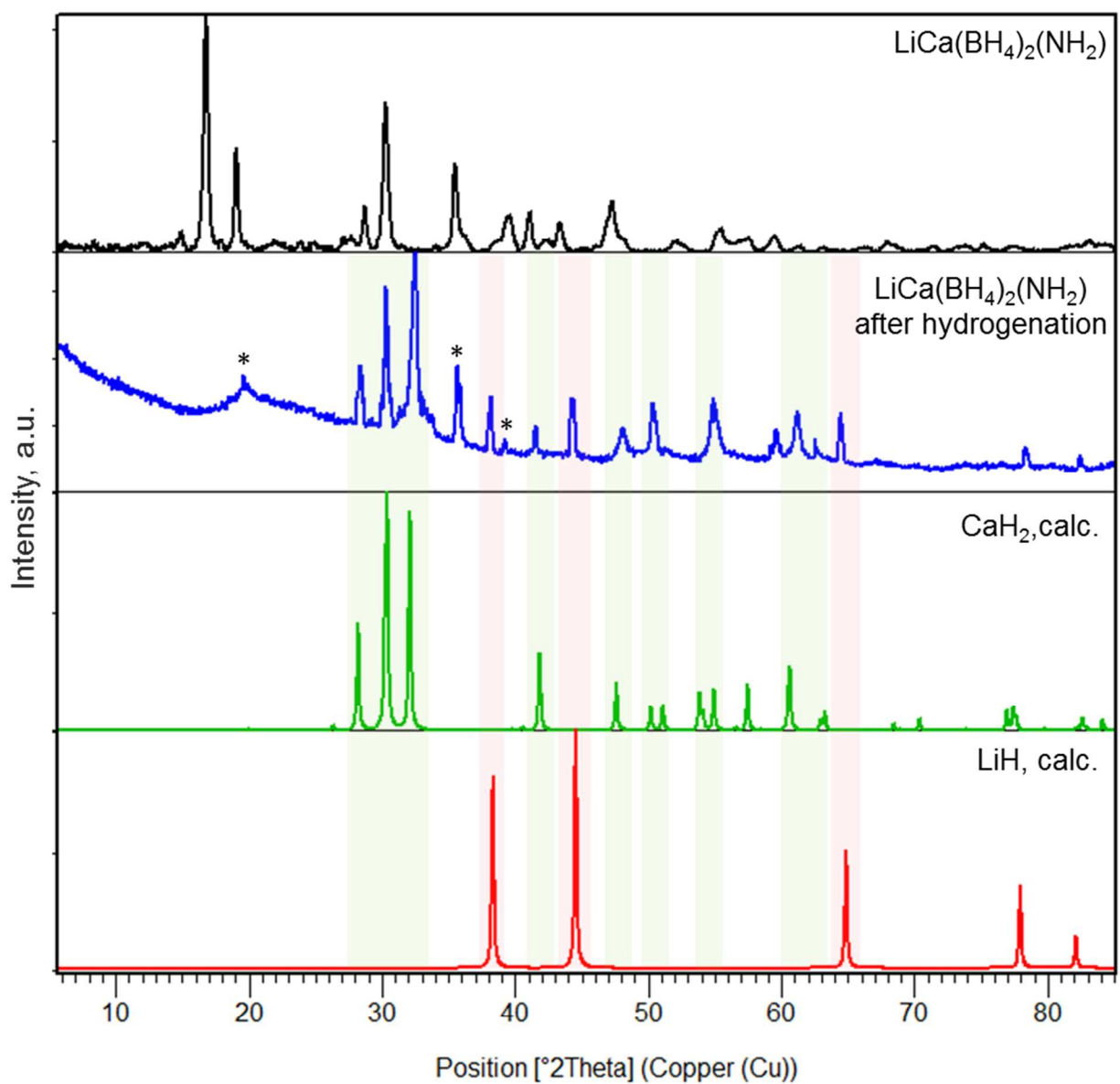


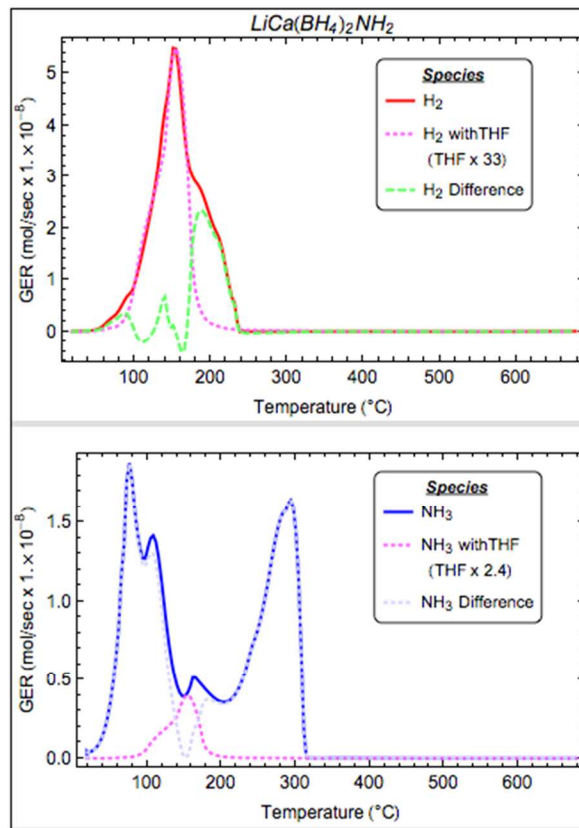
Figure S1. Schematic representation of the STMBMS apparatus.



**Figure S2.** XRD patterns of  $\text{Ca}(\text{BH}_4)_2 + \text{MNH}_2$  systems, where  $M = \text{Li}, \text{Na}$  along with their starting materials and possible metathesis products.



**Figure S3.** XRD patterns of as synthesized  $\text{LiCa}(\text{BH}_4)_2(\text{NH}_2)$ , rehydrogenated  $\text{LiCa}(\text{BH}_4)_2(\text{NH}_2)$  (under 106 bar  $\text{H}_2$  pressure at 230 °C) in comparison with the calculated patterns of  $\text{CaH}_2$  and  $\text{LiH}$ . The diffraction peaks corresponding to an unidentified phase (at 19.4°, 35.7° and 39.2°) are marked with asterisks.



**Figure S4:** STMBMS data examining the initial release of hydrogen (top) and ammonia (bottom) from  $\text{LiCa}(\text{BH}_4)_2(\text{NH}_2)$ . Both hydrogen and ammonia release associated with  $\text{LiCa}(\text{BH}_4)_2(\text{NH}_2)$  are reported as the dotted difference curve, identifying gas release not associated with THF emission.