Discovery and Development of Metal Hydrides for Reversible On-board Hydrogen Storage

Mark Allendorf and Vitalie Stavila

Sandia National Laboratories
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Project ID: ST033

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Overview of Sandia Program

**Timeline**
- Project started in March ‘05
- Project end June 2010
- Percent complete 100%

**Barriers**
- A. System Weight & Volume, B. Cost, C. Efficiency, D. Durability
- E. Charge/discharge rates
- P. Lack of Understanding of Hydrogen Physisorption and Chemisorption

**SNL R&D Budget**
- FY08 Funds: $2.4M
- FY09 Funds: $3.1M
- FY10 Funds: $1.9M

**MHCoE Partners**
- BNL, JPL, NIST, ORNL, SRNL, Caltech, GA Tech, OSU, PITT, Stanford, UH, UIUC, UNR, UNB, Utah, HRL, UTRC

**Collaborators**
- V. Ozolins (UCLA), J. Herberg (LLNL), Y. Filinchuk (ESRF), C. Wolverton (Northwestern), J-H Her (U. Maryland)
Technical POC and MHCoE Director: Lennie Klebanoff

Core Technical Team

Mark Allendorf: Theory, Theory Group Coordinator
Eric Majzoub: PEGS theory, experiments (Sandia/UMSL)
Vitalie Stavila: New materials (borohydrides, ammine complexes)
Joe Cordaro: New materials (P materials, bulk syntheses)
Weifang Luo: New materials (Li-N-Mg-H materials)
Mitch Anstey: P-containing materials

Other Key Contributors

Rich Behrens, Ida Nielsen

Ph.D. Students

Rebecca Newhouse, Leo Seballos (UC Santa Cruz),
Godwin Severa (U. Hawai’i), David Peaslee (UMSL)

Undergraduate Student

Natchapol Poonyayant (Mahidol University, Thailand)
Discover, develop and validate “reversible” on-board metal hydride storage materials with potential to meet the DOE 2010 targets and a clear path to meeting the 2015 targets. Use theory-directed synthesis and characterization

**Prediction of crystal structures:**
- Prototype Electrostatic Ground State (PEGS) technique for structure predictions and rapid $\Delta H$ estimates
- First-principles Density Functional Theory (DFT) is used for accurate thermodynamics calculations

**Synthesis/sample preparation:**
- Solid-state and solution routes
- High-energy ball-milling (SPEX), cryo-milling
- Hot-sintering at high-P (600 C, 2000 bar)

**Understanding structural properties / Probing reaction mechanisms / Additives/dopants/catalysts modification:**
- Powder/Synchrotron XRD, Neutron diffraction, STMBMS, PCT/Sieverts, Raman, FTIR, TGA/DSC, TEM, SEM, EDAX, EELS
Status of Theory in June 2009 and Current Focus

Theory Status in June 2009:

- Established Multiphase Equilibria (MPE) Theory:
  -- applied to LiNH$_2$ (+LiH); LiBH$_4$ /C
- Coordinated the MHCoE Theory Group (TG)
- Used PEGS to predict structures of LiSc(BH$_4$)$_4$, M-Ti(BH$_4$)$_x$, [B$_{12}$H$_{12}$]$^{2-}$
- Predicted $\Delta$H dehydrogenation for borohydride destabilized reactions

Theory Focus During FY09/10:

- MPE Theory applied to LiBH$_4$ and the formation of Li$_2$B$_{12}$H$_{12}$
- MPE Theory applied to LiBH$_4$ + MgH$_2$: Pressure-dependent mechanism
- MPE Study of 2LiNH$_2$ + C $\rightarrow$ Li$_2$CN$_2$ + 2H$_2$, a rxn. predicted by MHCoE TG
- Mg(BH$_4$)$_2$ + 2C $\rightarrow$ MgB$_2$C$_2$ + 4H$_2$, another predicted destabilized Rxn.
- PEGS studies of Ti(BH$_4$)$_3$, M[PB$_2$H$_8$]$_x$ for M = Li, Na, K, Mg, Ca
- Continued Coordination of the MHCoE Theory Group
Thermodynamics of Both Gas-phase and Solid-state Chemistry are Needed

Phase equilibrium calculations can reveal complex hydride decomposition chemistry to better predict gas-phase and solid products...

Approach: DFT/Gibbs Free Energy Minimization

- Compute hydride thermodynamics
  - DFT: Ground-state energies (0 K)
  - PHONON: finite-temperature thermodynamics (C_p^o, S^o, ΔH^o)
  - Fit C_p^o to polynomial
- Compute equilibrium at constant T,P
  - FactSage package (commercial software)
  - Include all relevant gas- and solid-phase species:
    - Gas phase: JANAF Tables
    - B_xH_y - B_{19}H_{14}
    - Li-B-C-Mg crystalline phases
    - Some liquids
      \[ C_p = a + bT + cT^2 + dT^3 \]

\[
G = \sum_{\text{ideal gas}} n_i(g_i^o + RT \ln P_i)
+ \sum_{\text{pure condensed phases}} n_i g_i^o
\]
Representative MH systems considered to assess the importance of full-scale equilibrium

**MPE Theory Results Last Year:**
- LiNH₂ (+ LiH): NH₃, N₂ formation; thermodynamic vs. kinetic products
- LiBH₄ + C: Hydrocarbon formation

**MPE Theory Results This Year:**
- LiBH₄: Li₂B₁₂H₁₂ intermediate formation
- 2LiNH₂ + C → Li₂CN₂ + 2H₂, 31.4 kJ/mol H₂
- LiBH₄ + MgH₂: Pressure-dependent mechanism*
- Mg(BH₄)₂ + 2C → MgB₂C₂ + 4H₂, 43.1 kJ/mol H₂*

* -- see our additional slides
LiBH$_4$: condensed-phase intermediate formation

- Predicted overall reaction:
  LiBH$_4$ $\rightarrow$ 1/12(Li$_2$B$_{12}$H$_{12}$) + 5/6LiH + 13/12H$_2$ (426K)

- Small kinetic barrier suggested
  - 440 K onset Kostka et al., P$_{tot}$ = 10$^{-6}$ mbar
  - $\sim$ 600 K Pinkerton et al., P$_{tot}$ = 1 atm

- B$_2$H$_6$ formation:
  - Detected by Kostka et al. (JPCC 2007)
  - B$_2$H$_6$(g) is not stable; converts to B$_x$H$_y$
  - B$_2$H$_6$ probably not detectable at 1 atm

- Effect of nanoconfinement
  - Gross et al. no Li$_2$B$_{12}$H$_{12}$ (JPCC 2008)
  - Li$_2$B$_{12}$H$_{12}$ stability reduced?
  - Alternative kinetic pathway?
Carbon Destabilization: LiNH$_2$ + 0.5C

MHCoE TG Prediction (Alapati et al. (JPCC 2008))

$$2\text{LiNH}_2 + \text{C} \rightarrow \text{Li}_2\text{CN}_2 + 2\text{H}_2 \quad \Delta U(0 \text{ K}) = 31.4 \text{ kJ/mol H}_2$$

Reactions predicted by MPE Theory:

- LiNH$_2$ + 0.5C $\rightarrow$ 0.4LiNH$_2$ + 0.3Li$_2$CN$_2$+0.25H$_2$+0.2CH$_4$ (T < 350 K)
- LiNH$_2$ + 0.5C $\rightarrow$ 0.5Li$_2$CN$_2$+H$_2$ (T > 350 K)

-- CH$_4$ predicted to be a major gas-phase by-product for H$_2$ release below 350 K

-- Li$_2$CN$_2$+H$_2$ are predicted to be major products at T > 350 K, avoiding CH$_4$ formation
## All Theory Milestones Are Complete

<table>
<thead>
<tr>
<th>Month/year</th>
<th>Milestone or Go/No-Go decision: Al-Adduct Theory, MPE Theory</th>
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<tbody>
<tr>
<td>May-08 ✓</td>
<td>Milestone: Complete BAC calculations of alane-amine complexes</td>
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<tr>
<td>Sep-08 ✓</td>
<td>Milestone: Complete BAC calculations on alane-adduct complexes</td>
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<tr>
<td>Dec-08 ✓</td>
<td>No-go: Model reactions of alane-amine surface interactions</td>
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<tr>
<td>May-09 ✓</td>
<td>Milestone: Complete calculations on alanate-amine complexes</td>
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<tr>
<td>Sep-09 ✓</td>
<td>Milestone: Complete calculations on alanate-ether adducts</td>
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<tr>
<td>Apr-10 ✓</td>
<td>Milestone: Evaluate gas-phase species formation in C-containing materials</td>
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<tr>
<td>Jun-10 ✓</td>
<td>Milestone: Evaluate gas-phase species formation in B-containing materials</td>
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<tr>
<th>Month/year</th>
<th>Milestone or Go/No-Go decision: Borohydride Theory</th>
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<tr>
<td>Oct-09 ✓</td>
<td>Milestone: Complete PEGS searches for new high-H₂ content mixed alkali-TM borohydrides</td>
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<tr>
<td>Feb-09 ✓</td>
<td>No-go: Discontinue surfactant templating for nano-scale alanates/borohydrides</td>
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<tr>
<td>Mar-10 ✓</td>
<td>Milestone: Complete PEG searches for new mixed cation alkaline-earth TM borohydrides</td>
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<tr>
<td>May-10 ✓</td>
<td>Go/no-go: Discontinue alkali-TM borohydrides if no suitable materials found</td>
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Discovery and Characterization of New Materials

Status in June 2009:

- Completed Ca(BH$_4$)$_2$, made “downselect” decision (no further work)
- Synthesized and characterized ammine adducts of borohydrides
- Synthesized and examined closo-borates ([B$_{12}$H$_{12}$]$^2$-) predicted by PEGS
- Initiated work on P-based hydrogen storage materials

**Final Year Goals:** Improve our understanding of high wt. % borohydrides, find new materials based on P and optimize 2LiNH$_2$/MgH$_2$ -- recommended by the MHCoE to the HSECoE as a preferred “near-term” material.

- Additive studies of Mg(BH$_4$)$_2$
- Destabilization of CaB$_{12}$H$_{12}$ with CaH$_2$
- Rehydrogenation of Li$_2$B$_{12}$H$_{12}$ and Na$_2$B$_{12}$H$_{12}$
- Hydrogen storage properties of P-containing metal hydrides
- Catalysis of 2LiNH$_2$/MgH$_2$ by KH and KNH$_2$
- Synthesized and characterized Ti(BH$_4$)$_3$ -- see additional slides
**TiF$_3$/ScCl$_3$ Enhances H$_2$ Desorption from Mg(BH$_4$)$_2$**

Desorption of Mg(BH$_4$)$_2$ ball-milled with 5mol % TiF$_3$ and 5mol% ScCl$_3$

- Small amounts of boron hydrides (15 – 58 amu) (<0.2wt%) are released
- Other transition metal chlorides (Mn(II), V(III), Ni(II) and Cu(II)) alone or in combination with Ti(III) and Sc(III) salts were not as effective as TiF$_3$/ScCl$_3$
- The transition metal additives generally degrade reversibility.

---

R. Newhouse, V. Stavila, S. Hwang, L. Klebanoff, J.Z. Zhang

Understanding \([B_{12}H_{12}]^{2-}\) Intermediates

\[
\text{CaB}_{12}\text{H}_{12} \rightarrow \text{CaB}_6 + 6\text{B} + 6\text{H}_2 \quad \Delta H (0\text{K}) = 65 \text{ kJ/moleH}_2 \quad ; \quad T(1\text{bar}) = 306 \text{ C}
\]

\[
\text{CaB}_{12}\text{H}_{12} + \text{CaH}_2 \rightarrow 2\text{CaB}_6 + 7\text{H}_2 \quad \Delta H = 38.6 \text{ kJ/moleH}_2 \quad ; \quad T(1\text{bar}) = 86 \text{ C}
\]

-- predicted by Ozolins, Majzoub and Wolverton, JACS, 2009, 131, 230.

Experimentally, we see no \(H_2\) release from \(\text{CaB}_{12}\text{H}_{12}\) heated to 700 \text{ C}.

\(\text{CaB}_{12}\text{H}_{12} + \text{CaH}_2\) releases \(H_2\) at \(~500 \text{ C}\).

The presence of \(\text{CaH}_2\) decreases the \(T\) required to release \(H_2\) from \(\text{CaB}_{12}\text{H}_{12}\) by > 200 \text{ C}, in good agreement with prior theory.

We also see a slight destabilization of \(\text{Li}_2\text{B}_{12}\text{H}_{12}\) and \(\text{Na}_2\text{B}_{12}\text{H}_{12}\) by \(\text{MgH}_2\)
Reversibility of Li$_2$B$_{12}$H$_{12}$, Na$_2$B$_{12}$H$_{12}$ Demonstrated at High H$_2$ Pressure

p(H$_2$) = 70–90 MPa (>10,150 psi), t = 400–500 C, reaction time: 16–72 hours

[B$_{12}$H$_{12}$]$^2^-$ compounds can be converted quantitatively into borohydrides in the presence of the corresponding metal hydride at high H$_2$ pressure. Conclusion confirmed by solid-state NMR (Caltech) and neutron vibrational spectroscopy (NIST).
Bis(borano)hypophosphites

Bis(borano)hypophosphites are:

- Air and water tolerant
- Soluble in most organic solvents
- Form concentrated solutions/gels
- Theoretical Weight % of H₂ is 8-12 %

Previous synthetic methods used PH₃, PH₃-BH₃, or PH₄I as the source of phosphorus, which are dangerous precursors.

We developed a safe route to M[PB]ₓ Na[PB], Na[PB]-d8, Li[PB], and Ca[PB]₂.
Na[PB] Structure Understood Theoretically, Experimentally

Identity of the anionic species confirmed by solution NMR

PEGS Predicted Crystal Structure in Agreement with Experiment
Na[PB] Thermal Decomposition

- ~ 6 wt. % H₂ desorbed from the Na[PB] material
- Reasonable H₂ desorption temperature of ~165°C is observed
- Faster heating rates yield more endothermic melting, slower heating rates favor exothermic H₂ release.
- Attempts to rehydrogenate desorbed material have so far been unsuccessful

Simultaneous Thermogravimetry Modulated Beam Mass Spectrometry (STMBMS):

- Release of PH₃ and B₂H₆ combined with lack of reversibility lead us to downselect Na[PB], removing from further consideration.
Further Work on $2\text{LiNH}_2/\text{MgH}_2$

$2:1 \text{LiNH}_2/\text{MgH}_2$

$2\text{LiNH}_2 + \text{MgH}_2 \rightarrow \text{MgLi}_2(\text{NH})_2 + 2\text{H}_2 - \text{H}_2 + 2\text{H}_2$

Mg($\text{NH}_2$)$_2 + 2\text{LiH}$

5.0 wt% shown


-- honored as a “Top Cited” paper by this journal in 2009

-- recommended by the MHCoE as a “near term” material for the HSECoE

- Potassium doping dramatically improves absorption rate.
- $\Delta H_{\text{des.}} = 42$ kJ/mole $\text{H}_2$
- Proven reversible hydrogen capacity of 5wt%, 1wt% more than NaAlH$_4$
- Excellent Cyclability: 264 cycles demonstrated, with 23% loss in capacity
- Manageable NH$_3$ release (200 ppm at 180 °C), but needs improvement

More capacity possible with $1:1 \text{LiNH}_2/\text{MgH}_2$ material, but need to improve pressure of 1st plateau region, cyclability
KH, KNH₂ Promote Absorption Kinetics of 2LiNH₂+MgH₂

Motivation: P. Chen et. al. show that KH can aid kinetics in Li-Mg-N-H systems (Angew. Chem. Int. Ed. 2009, 48, 1-5)

Our Work: Both KH and KNH₂ aid absorption kinetics (K⁺ catalytic agent)

KH (4mol%) improves absorption rate

KH dramatically aids absorption kinetics

Comparison of desorption profiles

Little catalytic effect on desorption

ΔHₜₐₚₔ = 42 kJ/mole H₂

--- results support prior work by Chen. et. al
## Experimental Milestones Are Completed

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<th>Month/year</th>
<th><strong>Milestone or Go/No-Go decision</strong></th>
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</table>
| Jan-09 ✓   | Milestone: Synthesize Ca(BH₄)₂/NH₃ system  
No-go: On further work on Ca(BH₄)₂/NH₃ system  
Milestone: Complete STMBMS characterization of Ca(BH₄)₂ |
| Mar-09 ✓   | Milestone: Lowering of Ca(BH₄)₂ desorption temperature  
No-go decision made on Ca(BH₄)₂ |
| June-09    | Go/no-go: Continue with mixed Ca₁₋ₓMₓ(BH₄)ₓ materials if reversibility has been shown at improved P and T compared to Ca(BH₄)₂ : No-Go Decision Made |
| Sep-09 ✓   | Milestone: Incorporation of hydride material in catalyzed nano-frameworks |
| Dec-09 ✓   | Isolate and assess the H₂ storage properties of new mixed cation alkali-TM borohydrides |
| Dec-09 ✓   | Synthesize and characterize NaPB₂H₈ and LiPB₂H₈. |
| Jan-10 ✓   | Complete mechanistic study of the hydrogenation/dehydrogenation of LiMgN |
| Feb-10 ✓   | Go/no-go on A-TM-(BH₄)ₓ : No-Go decision made on alkali transition metal borohydrides |
| Apr-10 ✓   | Characterize the H₂ desorption properties of modified Mg(BH₄)₂ |
| Apr-10 ✓   | Determine the H₂ desorption properties of NaPB₂H₈ and LiPB₂H₈ |
| Apr-10 ✓   | Synthesize and characterize Mg[PB₂H₈]₂ and Ca[PB₂H₈]₂ |
Summary of Accomplishments

**Theory:**

Gained a better mechanistic understanding of H\textsubscript{2} release and the role of impurity gas formation in high wt. % borohydride and amide materials:

\[
\text{LiBH}_4, \text{LiBH}_4/\text{MgH}_2, 2\text{LiNH}_2/\text{C}, \text{Mg(BH}_4)_2/\text{C}
\]

Predicted MH structures, allowing DFT calculations of reaction thermodynamics:

\[
\text{Ti(BH}_4)_3, \text{Li}_2\text{MgN}_2\text{H}_2, \text{LiPB}_2\text{H}_8, \text{NaPB}_2\text{H}_8, \text{KPB}_2\text{H}_8, \text{Mg}[\text{PB}_2\text{H}_8]_2, \text{Ca}[^\text{PB}_2\text{H}_8]_2
\]

Successfully Coordinated the MHCoE Theory Group

**New Materials:**

- Improved the desorption kinetics of Mg(BH\textsubscript{4})\textsubscript{2}
- Developed a route for releasing H\textsubscript{2} from B\textsubscript{12}H\textsubscript{12} compounds, confirmed prior theory
- Demonstrated hydrogenation of Li\textsubscript{2}B\textsubscript{12}H\textsubscript{12} and Na\textsubscript{2}B\textsubscript{12}H\textsubscript{12} at high H\textsubscript{2} pressure
- Successfully synthesized and characterized H\textsubscript{2} storage properties of NaPB\textsubscript{2}H\textsubscript{8}
- Confirmed remarkable catalysis of 2LiNH\textsubscript{2}/MgH\textsubscript{2} by KH and KNH\textsubscript{2}
- Successfully synthesized and characterized Ti(BH\textsubscript{4})\textsubscript{3}
Collaborations

**MHCoE Partners:**
- BNL: J. Wegrzyn, J. Graetz
- Caltech: S.-J. Hwang, C. Ahn
- HRL: J. Vajo, P. Liu
- GA Tech: D. Sholl
- JPL: J. Reiter, J. Zan
- NIST: T. Udovic, U. Kattner
- OSU: J.-C. Zhao
- SRNL: D. Anton, R. Zidan
- U. Hawai’i: C. Jensen
- U. Illinois: I. Robertson, D. Johnson
- UNR: D. Chandra
- U. Pitt: K. Johnson
- U. Utah: Z. Fang
- UTRC: X. Tang, D. Mosher, S. Opalka

**Other Collaborations:**
- ESRF: Y. Filinchuk
- LLNL: J. Herberg
- Northwestern: C. Wolverton
- UCLA: V. Ozolins
- U. Maryland: J.-H. Her
Additional Slides
2LiBH$_4$ + MgH$_2$: pressure-dependent mechanisms

$P_{tot} = 1$ atm H$_2$ (2-step mechanism):
- LiBH$_4$ → 1/12(Li$_2$B$_{12}$H$_{12}$) + 5/6LiH + 13/12H$_2$
- Li$_2$B$_{12}$H$_{12}$ + 6MgH$_2$ → 2LiH+6MgB$_2$+11H$_2$

100 atm H$_2$ (3-step mechanism):
- LiBH$_4$ → 1/12(Li$_2$B$_{12}$H$_{12}$) + 5/6LiH + 13/12H$_2$
- MgH$_2$ → Mg + H$_2$ (782 K)
- Li$_2$B$_{12}$H$_{12}$ + Mg → LiH+MgB$_2$ + H$_2$

→ Kinetic limitation to Li$_2$B$_{12}$H$_{12}$ determines decomposition
→ Li$_2$B$_{12}$H$_{12}$ is thermodynamically ‘destabilized’ in the presence of MgH$_2$
Mg(BH$_4$)$_2$ (+ 2C): thermodynamic and kinetic effects

\[ \text{Mg(BH}_4\text{)}_2 + 2\text{C} \rightarrow \text{MgB}_2\text{C}_2 + 4\text{H}_2 \]
\[ \Delta U(0 \text{ K}) = 43.1 \text{ kJ/mol H}_2 \]

- Newhouse et al. *JPCC* 2010
  - $T_{\text{onset}} = 540$ K
  - MgB$_{12}$H$_{12}$ is detected

- Thermodynamic advantage to C addition as well as kinetic

- Nanoconfinement
  - Infiltrated C aerogel reduces $E_a$
  - H$_2$ release suggests no CH$_4$ forms


Fichtner et al., *Nanotechnology*, 2009, 204029.
Alkali and Alkaline Earth Borano-hypophosphite

Stability Trends Assessed Using PEGS*-generated Crystal Structures

- Several high symmetry candidates identified
- Preliminary stability of the salts indicates: Na < Li < K; Ca < Mg

Highly-ordered Nano-porous Templates

Synthesis From Block-polymer And Cross-linked Phenolic Resins

Advantages:
- versatile and easily controlled mesostructure
- narrow pore size distribution
- large volumes: 0.8 cc/g
- tunable pore size: 2-20 nm
- resol polymer template OR carbon-only template
- variety of morphologies
- potentially monolithic


Templates are being used for Mg(BH₄)₂, Ca(BH₄)₂ infiltration
Developed Method to Convert $2\text{LiNH}_2/\text{MgH}_2$ into $2\text{LiH} + \text{Mg(NH}_2)_2$

Exothermic process from conversion of

$2\text{LiNH}_2+\text{MgH}_2 \rightarrow 2\text{LiH}+\text{Mg(NH}_2)_2$

H$_2$ release at different temperatures

$2\text{LiH} + \text{Mg(NH}_2)_2$ demonstrates cleaner H$_2$ desorption, and lower T (which also helps suppress NH$_3$ formation)
Absorption kinetics of MgLi$_2$(NH)$_2$/KH

KH aids the absorption kinetics of the 2LiNH$_2$/MgH$_2$ material system
Mg\((BH_4)_2\) Compositional Studies with SEM/EDX

- Mg\((BH_4)_2\), 600 °C
- Mg\((BH_4)_2\) + additives, 600 °C

MgB\(_2\) almost exclusively formed upon heating up to 600 °C.

Additives are distributed relatively uniformly throughout the boride sample.
Dehydrogenation from Ti(BH$_4$)$_3$ occurs between 22 °C < T < 140 °C.

Problems include poor reversibility, and gas-phase impurities (B$_2$H$_6$ / H$_2$ ~ 1:100).

Partial electronic density of states for Ti(BH$_4$)$_3$. Yellow spheres represent Ti, which is coordinated to the [ BH$_4$ ]$^-$ anions. The partial DOS indicate Ti-H d-s hybrid orbital.

- Theory shows that Ti(BH$_4$)$_4$ is unstable with respect to decomposition into Ti(BH$_4$)$_3$.
- Ti(BH$_4$)$_3$ predicted to be unstable at RT (in agreement with expt.).

Na[PB] Thermal Decomposition

- ~6 wt. % H₂ desorbed from the Na[PB] material
- Reasonable H₂ desorption temperature of ~165°C is observed
- Faster heating rates yield more endothermic melting, slower heating rates favor exothermic H₂ release.
- Attempts to rehydrogenate desorbed material have so far been unsuccessful

Melting and decomposition occur near the same temperature; more decomposition means less Na[PB] left to melt, smaller endothermic peak
STMBMS*: A New MHCoE Capability to Elucidate Complex Reaction Processes

* Simultaneous thermo-gravimetric modulated-beam mass spectrometer

This instrument, developed for our national security work, is used to study reaction kinetics of complex systems

Instrument details:
- Knudsen effusion cell installed within a furnace and upon a microbalance
- Simultaneous modulated molecular beam mass spectrometer provides time-dependent species info
- High accuracy FTMS for species identification

Data:
- Species
- Number density
- Rate of evolution
- Partial pressure
- Temperature

Data is correlated and analyzed to determine reaction processes and kinetics