Metal Hydride Center of Excellence

Lennie Klebanoff, Director (presenting)

Jay Keller, Sandia Hydrogen Program Manager

http://www.ca.sandia.gov/MHCoE/

(This presentation does not contain any proprietary information)

Agenda for Tech Team Review

1. *MHCoE Overview (20 mins):* Lennie Klebanoff
2. *MHCoE Theory (60 mins):* David Sholl
3. *Metal Borohydrides (75 mins):* Ewa Rönnebro and Craig Jensen
4. *AlH_3 (60 mins):* Jason Graetz, Craig Jensen, Ragaiy Zidan
5. *Amides (60 mins):* Zak Fang
6. *Nanoconfinement /Destabilization (70 mins):* John Vajo
7. *Summary and Future Directions (15 mins):* Lennie Klebanoff

MHCoE Overview Outline

- *MHCoE Objectives*
- *Approach to Technical Targets*
- *Overall MHCoE Structure and Participants*
- *Comings and Goings*
- *2007 Materials Downselect Milestone, Criteria and Report*
- *By the Numbers…*
- *Critical Issues Addressed Today*

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MHCoE Objectives

Research, develop and validate reversible on-board metal hydride storage materials and systems that meet the 2010 DOE system targets for hydrogen storage, with a credible path forward for meeting the 2015 DOE storage targets

Approach to Technical Targets

H Capacity: 2010 System Targets: 6 wt. %, 45gH_2/L vol. density

- Synthesize and characterize hydride materials with high hydrogen capacity and favorable thermodynamics. Use state-of-the-art theory to guide materials discovery effort.

Charge/Discharge Rates: 2010 Sys. Target: 3 min. system fill (5kg)

- Develop materials that are fully reversible, catalysts that aid reversibility, assess nanoengineering promotion of kinetics, and investigate role of contamination on reaction rates

Hydrogen Purity (from Storage) : 2010 Target: 99.99% pure

- Assess release of NH_3, B_2H_6 and other volatile species from metal hydrides during desorption and cycling

Cycle Life: 2010 Target: 1000 Desorption/Adsorption Cycles

- Investigate durability of materials, cycling behavior, effects of contaminants, structural stability, release of volatiles

MHCoE Project Structure

DOE

Coordinating Council (2007-2008)

Bruce Clemens (Stanford, POC A), Ewa Rönnebro (SNL, POC B), Zak Fang (Utah, POC C), Jim Wegrzyn (BNL, POC D), Don Anton (SRNL, POC E), Craig Jensen (UH), Jay Keller (SNL) and Lennie Klebanoff (SNL)

Project Groups

A

Destabilized Hydrides

- **Stanford (POC)**
- Caltech
- JPL
- UIUC
- U. Hawaii
- U. Pitt/CMU
- HRL
- U. Utah
- Intematix
- NIST

B

Complex Anionic Materials

- **SNL(POC)**
- GE
- U. Hawaii
- UIUC
- JPL
- ORNL
- NIST
- UNR
- Utah
- UTRC

C

Amides/ Imides (M-N-H)

- **Utah (POC)**
- GE
- UNR
- ORNL
- U. Hawaii
- JPL
- Caltech
- SRNL

D

Alanes (AlH_3)

- **BNL(POC)**
- SRNL
- U. Hawaii
- SNL
- UIUC
- UNB

E

Engineering Analysis & Design

- **SRNL(POC)**
- NIST
- JPL
- GE
- SNL

MHCoE Budget: ~ $8.6M FY'07

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Comings and Goings

Welcome New Partners: (current total 19)

- UTRC (Dan Mosher, Sarah Arsenault, Susanne Opalka, and Xia Tang ---Project B)
- University of New Brunswick (Sean McGrady, Proj. D)
- The Ohio State University (J.-C. Zhao, Project B), pending
- Georgia Tech (David Sholl, Theory Group), pending
- Lawrence Livermore National Lab (Ted Baumann), TBD

Goodbye Former Partners, and thank you!

- GE (J.-C. Zhao moved to OSU)
- Carnegie Mellon University (David Sholl moved to GT)
- Intematix (Jonathan Melman, Darshan Kundaliya), leaving 6/2008

Materials Downselect Criteria

The MHCoE is focusing on 5 primary performance criteria on which Go/No-Go materials decisions were based:

1) **The material's hydrogen storage gravimetric density should be at least 5 weight percent**
2) **The material should be at least 50% reversible after 3 cycles**
3) **The material should release its H_2 for temperatures below 350 °C**
4) **The material's non-H_2 volatilization products should not exceed 1000 ppm for a single thermal cycle**
5) **The material should release and reabsorb H_2 in less than 24 hours.**

These criteria were used as guidelines in determining if specific material systems had sufficiently promising characteristics to warrant further work. They were not applied with absolute rigidity, nor do they substitute for the full DOE system targets for on-board hydrogen storage.

Materials Downselect Report

- 51 materials systems have been investigated in the MHCoE. Of these 51 materials, 24 were downselected removing them from further study. 27 have satisfied the 5 performance metrics and are being studied further.

Materials No Longer Being Pursued:

MgH_2/Si: not reversible **X**

$2LiNH_2 + MgH_2$: wt. % limited to ~5% **X**

$Li_2Zn(BH_4)_4$: B_2H_6/H_2 ratio of 0.3 **X**

Materials Still Being Pursued:

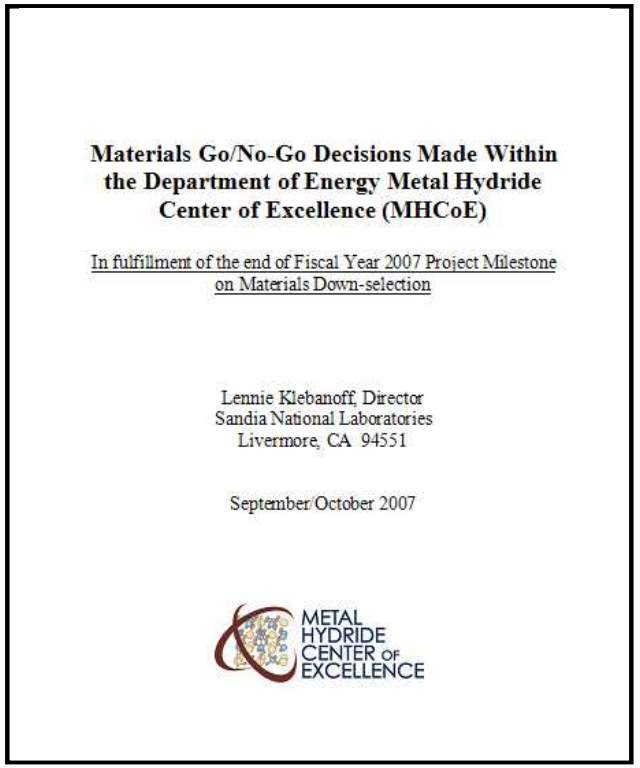
$Ca(BH_4)_2$ ✓

$LiBH_4/MgH_2$ in aerogels ✓

LiMgN, $Li_3AlH_6/3LiNH_2$ ✓

AlH_3 , and 22 other systems ✓

In fulfillment of the end of FY2007 Materials Downselect Milestone



Materials Go/No-Go Decisions Made Within the Department of Energy Metal Hydride Center of Excellence (MHCoE)

In fulfillment of the end of Fiscal Year 2007 Project Milestone on Materials Down-selection

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September/October 2007

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--- selected as a "Best Practices" Document by the DOE

By The Numbers….

From 3/2007 to 3/2008:

59 -- **MHCoE Publications (Published, Accepted, Submitted)***

→ **25** -- **Collaborative Publications (between partners)**

93 -- **MHCoE Talks**

4 -- **Patents filed based on MHCoE work**

***Published in:**

Phys. Rev. Lett. (3)	J. Inorg. Chem.
Phys. Rev. B	J. Alloys and Comp.
J. Amer. Chem. Soc.	J. Appl. Phys.
J. Phys. Chem. B, C	Scripta Materialia

Critical Issues Addressed Today:

Kinetics:

The adsorption/desorption kinetics of metal hydrides are typically too slow. Progress will be reported today in the use of nanoconfinement (**Vajo**) and catalysts (**Rönnebro**) to increase kinetic performance.

Thermodynamics:

The enthalpies of reaction and activation barriers for metal hydrides are typically too high, requiring desorption temperatures in excess of PEM fuel cell operating temperatures. Progress will be reported today in predicting new reaction schemes with favorable ΔH_{rxn} (**Sholl**), realizing those predicted materials (**Fang**), and studies of low-temperature reactions (**Jensen**).

Reversibility:

Many thermodynamically-promising metal hydride systems are either not reversible, or reversible only under impractical conditions. **Graetz, Jensen and Zidan** will report today on progress regenerating AlH_3 from Al, and **Rönnebro** will report on relaxing requirements for $Ca(BH_4)_2$ reversibility

… in addition to cycle life, H_2 capacity, hydrogen purity….

Overall Summary, Future Directions

..will be discussed after the technical presentations

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MHCoE Partners Meeting, December 11-12, 2007
Sandia National Labs, Livermore California

End of MHCoE Overview Presentation