METAL HYDRIDE CENTER OF EXCELLENCE

DOE Review, May 16, 2007

Metal Hydride Center of Excellence

Lennie Klebanoff, Director (presenting)

Jay Keller, Sandia H_2 Program Manager

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

(This presentation does not contain any proprietary information)

Project ID # STP30

MHCoE Overview Outline

- Overall MHCoE Structure, Participants
- Coordinating Council, Management Costs
- Center-wide, Project Milestone Tracking
- Projects A – E, Technical Highlights
- By The Numbers (summary of MHCoE pubs, talks, patents)
- Working Together
- Connections with Other Groups
- MHCoE Materials Relative to DOE Targets
- Closing the Gaps
- Overall MHCoE Future Direction

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MHCoE Project Structure

DOE

Coordinating Council (2006-2007)

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

Project Groups

A

Destabilized Hydrides

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

B

Complex Anionic Materials

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

C

Amides/ Imides (M-N-H)

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

D

Alanes (AlH_3)

- **BNL(POC)**
- SRNL
- JPL
- U. Hawaii
- SNL

E

Engineering Analysis & Design

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

Planned MHCoE Budget: $8.2M FY'07

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Coordinating Council

Purpose: Provide overall discussion/guidance to DOE on technical and programmatic directions, go/no-go decisions, center-wide issues

Current Activities:

- **Evaluating/Renewing Partner Phase I/Phase II Contracts**
- **Formulating Materials Down-Select Process for 9/2007 Milestone**
- **Improving Intellectual Property Procedures for the MHCoE**

The Council convenes many times per year, both telecons, face-face

Klebanoff, Keller are permanent members, with other positions evaluated yearly. Project POC's are also C.C. members

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MHCoE Mgmt. FY'07 Estimated Costs

Lead-Lab Center Mgmt. Cost: $445K total

$26.2K/partner (17 partners)

5.4% of MHCoE Budget

- DOE Interactions
- Coordinating Council
- MHCoE Milestones Tracking
- Center Meetings
- Partner Coordination
- Collaborations with Other Groups

Lead-Lab + Partners Mgmt. Cost: $625K total

$36.8K/partner

7.6% of MHCoE Budget

- All of the above, plus…..
- Project Meetings
- Developing/Tracking Project Milestones
- Coordinating Council
- Project-Project MHCoE Collaborations

Management and coordination of a large center is being provided at very reasonable cost

MHCoE Milestone Spreadsheet
-- Center-Wide Milestones --

As a Center we are organizationally tied to the MYRDDP Milestones

Milestone Level: MYRDDP, Center, or Project			Timeline begins FY05 (10/1/2004) and ends FY15 (9/30/2015). Each cell has a 6 month duration and starts on the day indicated.
Organization	Task #	Task Description	10/1 FY05 · 4/1 FY05 · 10/1 FY06 · 4/1 FY06 · 10/1 FY07 · 4/1 FY07 · 10/1 FY08 · 4/1 FY08 · 10/1 FY09 · 4/1 FY09 · 10/1 FY10 · 4/1 FY10 · 10/1 FY11
MYRDDP Milestones (Relevant to the MHCoE)			M, M, D
MHCoE Center Milestones			M, R, M, M, R, M, D
Task 4: R&D of Advanced Solid-State Materials for 2010 Targets (On-board Regeneration)			
CTR	Mat	Workshop for partners to present materials and show the council how their material or class of materials will meet the 2010 technical targets. (AUG 2007)	M — UPDATED
CTR	Mat	Prepare material classes for down selection & recommendations to DOE for redirection of resources to the top 50% (9/15/07)	R — UPDATED
DOE	7	Down-select on-board reversible metal hydride materials (4Q 2007)	M — UPDATED: moved back from 4Q FY09
CTR	Sys	Workshop for partners to present design engineering concepts and show the council how their concepts will meet the 2010 targets. (2Q 2009)	M — UPDATED
CTR	Sys	Prepare 2010 target based design concepts for down selection & recommendations to DOE for redirection of resources to the top 50%. (3Q 2009)	R — UPDATED
CTR	Sys	Complete proof of concept for a complex hydride integrated system meeting 2010 targets. (4Q 2010)	M
DOE	10	Go/No-Go: Decision on continuation of on-board reversible metal hydride R&D (4Q 2010)	UPDATED: moved back from 4Q FY12 — D
A. Destabilized Hydrides			D, D, D, D, D, D
B. Complex Anionic Materials (Borohydrides & Alanates)			D, D, D, D, D, D, D
C. Amide/Imides (M-N-H Systems)			D, D, D, D, D, D, D, D, D

MHCoE Milestone Spreadsheet
-- Project B Milestones --

Progress checked against milestones quarterly, aids planning, tracks technical risk, Rolls up to MYRDDP Milestones

Milestone Level: MYRDDP, Center, or Project			Timeline begins FY05 (10/1/2004) and ends FY15 (9/30/2015). Each cell has a 6 month duration and starts on the day indicated.													
Organization	Task #	Task Description	10/1	4/1	10/1	4/1	10/1	4/1	10/1	4/1	10/1	4/1	10/1	4/1	10/1	4/1
			FY05	FY05	FY06	FY06	FY07	FY07	FY08	FY08	FY09	FY09	FY10	FY10	FY11	FY11
B. Complex Anionic Materials (Borohydrides & Alanates)						D D	D	D	D	D				D		
	1	Modified Complex Hydrides			R					R				R		
	1.1	Development of alanates														
SNL-CA	1.1.1	Accomplish synthesis, characterization and measuring of sorption properties of a new bialkali alanate K2LiAlH6. Published in the Journal of Physical Chemistry B.			R											
U. Hawaii	1.1.2	Complete fundamental studies of the alanates. (Task completed)					R									
	1.2	Synthesis and characterization of borohydrides														
SNL-CA & U.	1.2.1	Synthesize high-capacity borohydrides in the solid state guided by the modeling efforts					M	M	M	R						
SNL-CA	1.2.2	Go/no-go for formation of Ca(BH4)2 and Mg(BH4)2. Go for Ca, no-go for Mg.				D D										
	D	Planned Portfolio Reallocation Decision Point (Project bars)														
	D	No Go decision / Resources reallocated to other materials														
	D	Go decision established														
	M	Milestone (Subtask bars)														
	R	Output (Task bars)														

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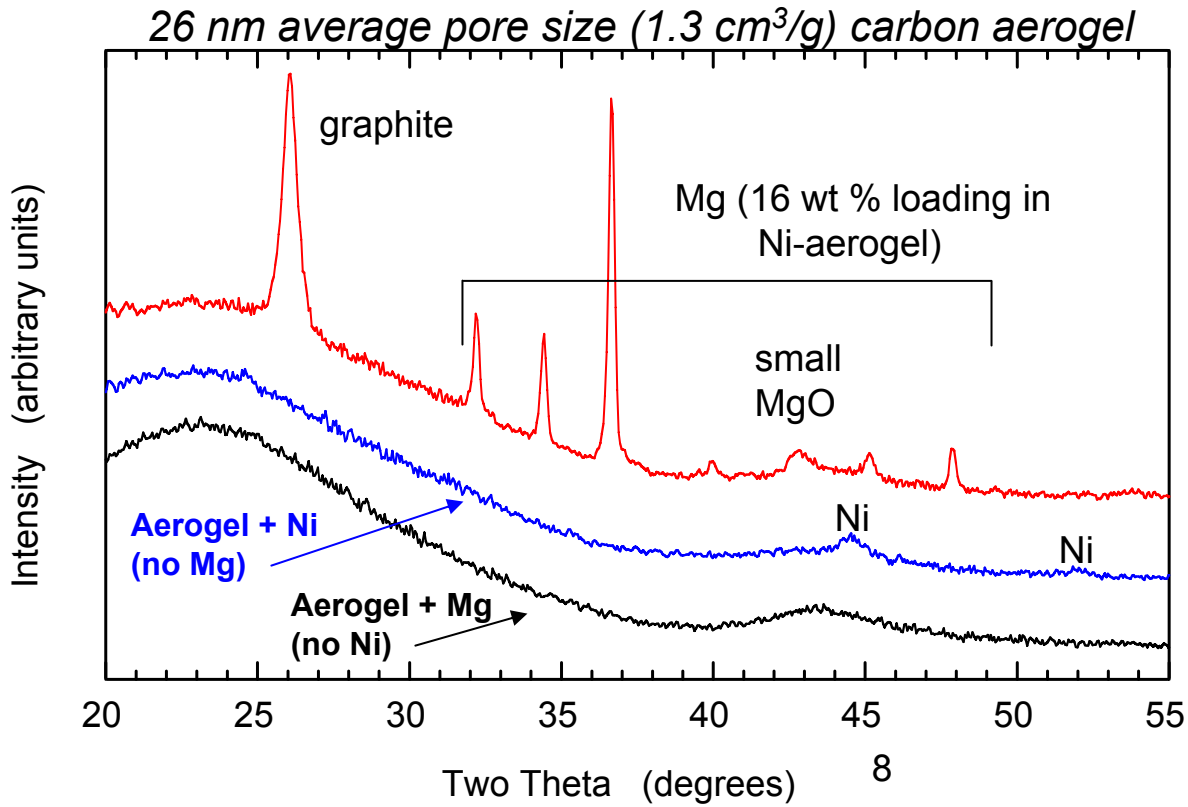
Project A – Destabilized Hydrides

Develop strategies for reducing H_2 storage thermal requirements, improve hydride kinetics

New Project Lead: Ian Robertson, UIUC

Project A Technical Highlight: **Nickel wetting layer enables incorporation of Mg into carbon aerogel**



-- See talk by:
Ping Liu (HRL)

Posters by:

Caltech
JPL
Stanford
Intematix
NIST

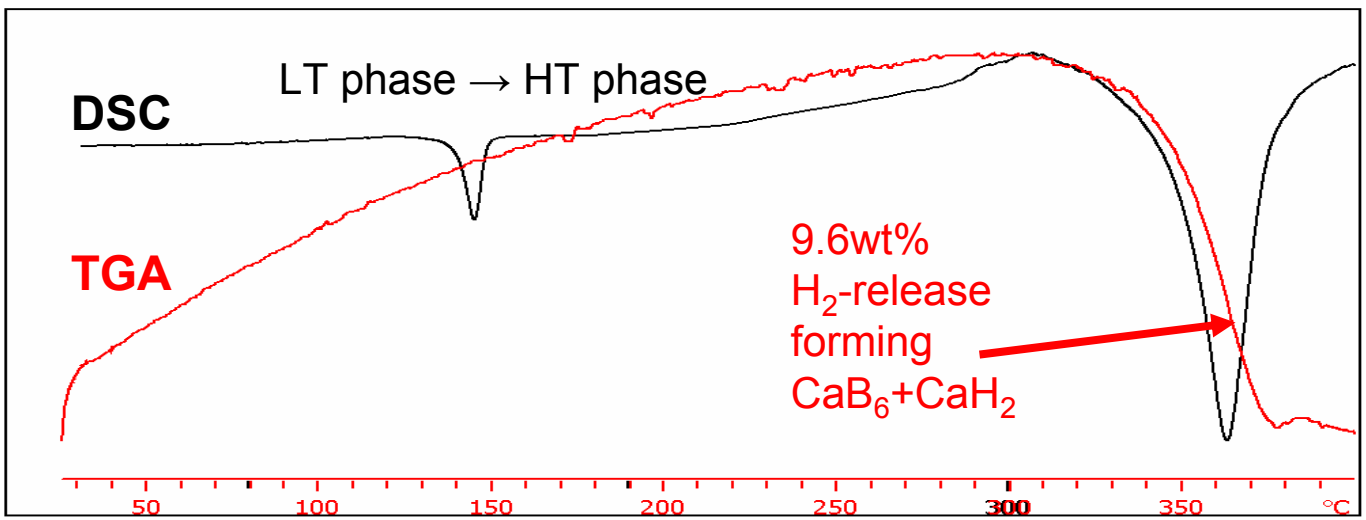
Project B - Complex Anionic Materials

Predict, synthesize and evaluate promising new complex hydride materials

Project Lead: Ewa Ronnebro, Sandia

Project B Technical Highlight: **Theory-predicted $Ca(BH_4)_2$ is reversible**

$CaB_6 + 2CaH_2 + 10\ H_2 \leftrightarrow 3Ca(BH_4)_2$ re-hydrided at 700bar, 400C



--- See Talk by:
Ewa Ronnebro (SNL)

Other talks by:
J.-C. Zhao (GE)
Craig Jensen (UH)
Karl Johnson (Pitt.)

Posters by:

UIUC, JPL
ORNL, NIST
Intematix
UNR, Utah

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Project C - Amides/Imides

Assess viability of amides, imides for on-board H_2 storage

New Project Lead: Zak Fang, U. Utah

Project C Technical Highlight:

$Li_3AlH_6/Mg(NH_2)_2$ can reversibly store ~ 6 wt% H_2 at T< 300°C. Reversibility confirmed by ^{27}Al NMR

2/3 Li_3AlH_6 + $Mg(NH_2)_2$

⇕

2/3 Al + $Li_2Mg(NH)_2$ + $3H_2$

(Dehydrogenated)

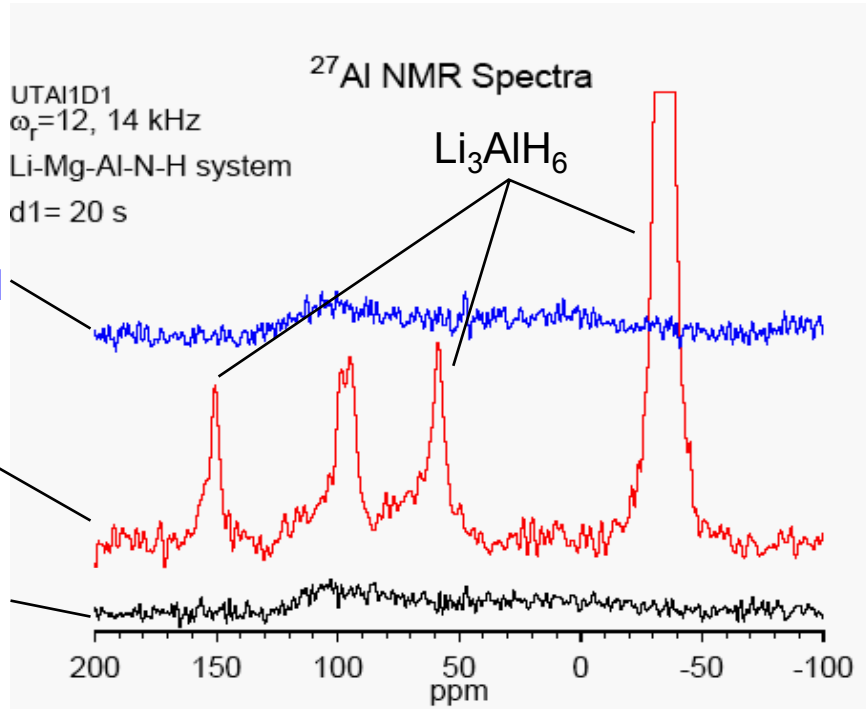
Dehydrogenated

↑

Hydrogenated

↑

Dehydrogenated



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Project D - Alane (AlH_3)

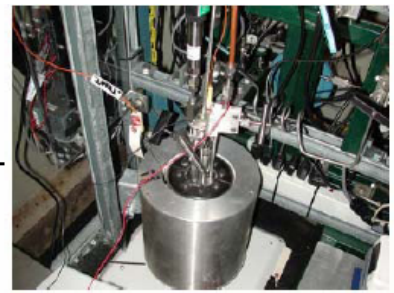
Understand desorption and regeneration properties of AlH_3 for H_2 storage

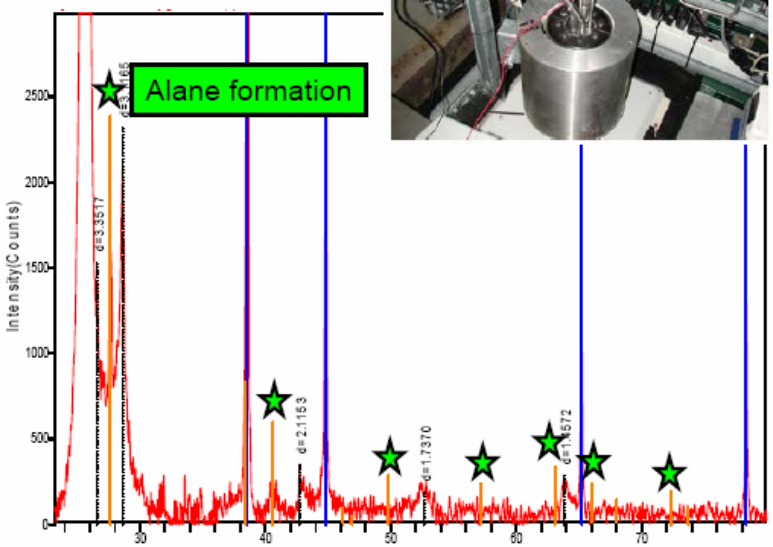
Project Lead: Jim Wegrzyn, BNL

Project D Technical Highlight: **Electrochem. Regeneration of Al → AlH_3**

- Electrochemical charging under elevated hydrogen pressure
- 500 psi H_2
- 60 C
- 10 V
- 2 hr

- Process needs to be optimized to increase yield from mg to g





--- for more results, see MHCoE Poster by Ragaiy Zidan (SRNL)

Also see talks by:
Jason Graetz (BNL)
Craig Jensen (UH)

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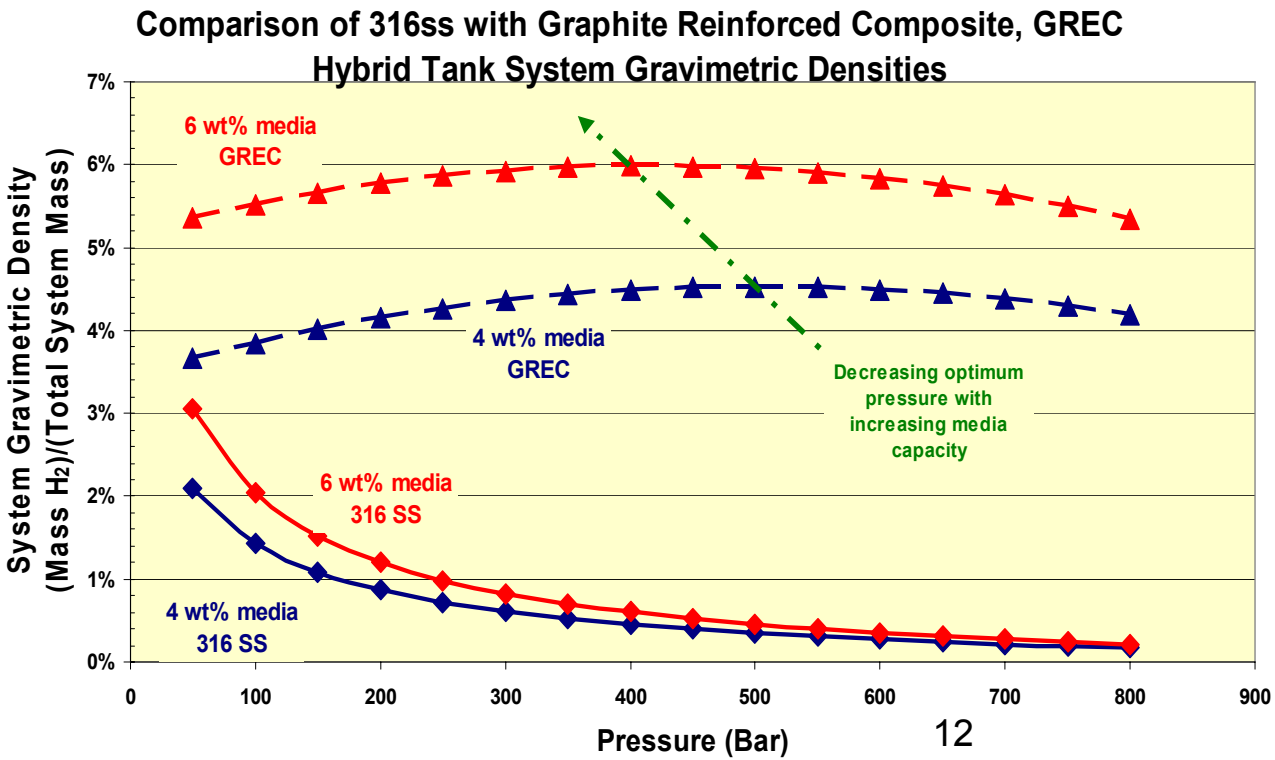
Project E: Eng. Design, Anal. and Test

Provide engineering, analysis and design supporting DOE system performance goals. Provide engineering-based materials targets

Project Lead: Don Anton, SRNL

Project E Technical Highlight: **MH/High Pressure Hybrid Tank Analyzed**



... Analysis reveals the effects of storage tank construction material, operating pressure, media gravimetric density and void fraction on system gravimetric and volumetric storage densities…

-- For more results, see poster by: Don Anton, SRNL

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By The Numbers….

From 5/2006 to 4/2007:

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

→ **20** -- Collaborative Publications (between partners)

87 -- MHCoE Talks

10 -- Patents filed based on MHCoE work

***Published in:**

Phys. Rev. Lett.	Inorg. Chem.	Scripta Materiala
Phys. Rev. B	J. Alloys and Comp.	J. of Metals
J. Amer. Chem. Soc.	J. Appl. Phys.	J. Solid State Chem
J. Phys. Chem. B, C	Acta Crysta	Chem. Materials

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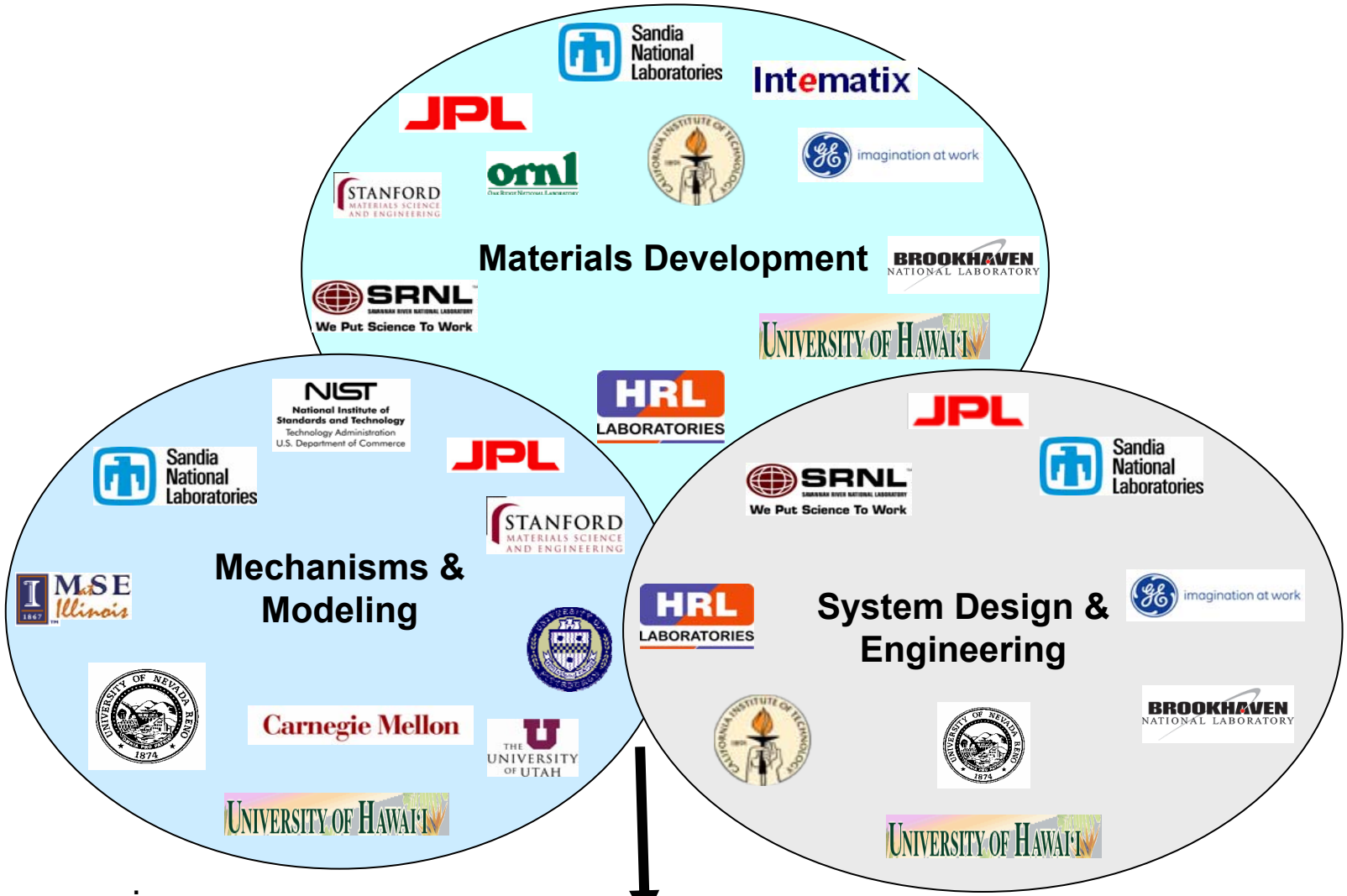
Working Together in the MHCoE



Teaming is occurring naturally due to organization in "project" space, see presentations

2010 System

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Theory Guides the MHCoE Materials Discovery Efforts

MHCoE Theory Group

Mark Allendorf (SNL, Coordinator), Duane Johnson (UIUC), Karl Johnson (Pitt.), Dave Sholl (CMU), Eric Majzoub (SNL), Ursula Kattner (NIST)

(Examples)

Sholl/Johnson (CMU/Pitt.)

$ScH_2 + 2LiBH_4$
$\Delta H \sim 34 kJ/mol\ H_2$

LiMgN

Ahn (Caltech)

Sc hydrogenation
$ScH_2/2LiBH_4$ prep.
H_2 desorption
^{45}Sc, ^{11}B, ^{7}Li, ^{1}H MAS-NMR

Bowman (JPL)

(Project A)

Fang (Utah)

Hydrogenation @ 138 bar/ 240°C,
^{6}Li, ^{1}H MAS NMR

Bowman (JPL)

(Project C)

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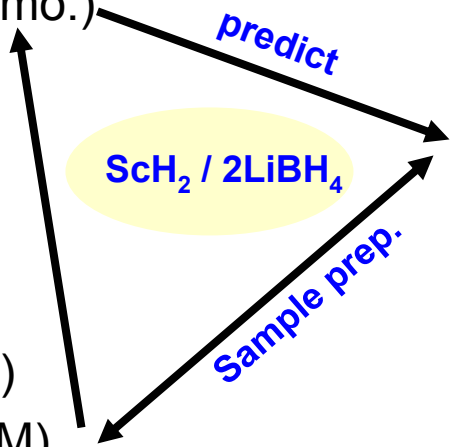
Working Together in Project A

Theory

CMU/U.Pitt/UIUC (Thermo.)
NIST (Phase diagrams)

Advanced Characterization

NIST (Neutron methods)
JPL/Caltech (NMR, TEM)
Stanford (Synchrotron XRD)
UIUC (*In situ* TEM)
SNL (High-P Sieverts system)



New Destabilized Systems

HRL ($LiBH_4$-based systems)
Pitt/CMU/UIUC (Theory/modeling)
Caltech/JPL (Ca alanate systems, $ScH_2 + 2(LiBH_4)$)
Hawaii (Work w/ UOP)
Utah (Li-Al-N syst.–mainly in Proj. C)

Kinetics

HRL (Nanostruct. materials, scaffolds)
Stanford (Thin-film model systems)
Intematix (Combinatorial – catalysts; nanoparticle synthesis)
Utah (High energy milling, CVS)
JPL/Caltech (T-ramp, RGA)
Hawaii (Novel catalysts)

" The MHCoE brought additional synthesis, characterization and modeling capabilities to the initial destabilization team, thereby accelerating this effort."
-- Ian Robertson, UIUC (Proj. A POC)

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Working Together in Project B

Theory, Modeling

SNL (MC, DFT)
UIUC (DFT)
Pitt (Kinetics)

predict

New Materials Synthesis

SNL ($Ca(BH_4)_2$, X-Ge-H, H.P.sintering, solvent, rapid screening)
GE ($Mg(BH_4)_2$, ball milling)
Hawaii (TM Borohydrides)
Utah (Mg mat.,Reactive milling)
ORNL ($Al(BH_4)_3$, Liq. Phase methods)

$Ca(BH_4)_2$

Ca-B-H samples

Advanced Characterization

SNL (XRD, Raman, DSC, TGA)
JPL/LLNL (NMR)
NIST (Neutron diffraction)
UIUC (TEM)
U. Nevada (In-situ XRD)
Intematix (Catalyst screening)
GE (Synchrotron in-situ XRD)

"The MHCoE enables metal hydride researchers to join forces towards finding new high-performance hydrogen storage materials"

-- Ewa Ronnebro, SNL (POC Project B)

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Working Together in Project C

Theory, Modeling

U.Pitt/CMU (DFT theory)
SNL (MC theory)

predict

New Materials Discovery

Utah (CVS, reactive milling)
ORNL (Wet Chemistry)

LiMgN

LiMgN Hydrogenation

Advanced Characterization

JPL (NMR, TEM)
GE (Synchrotron XRD)
UNR (PCT, cycling)
Hawaii (anelastic spect.)
SNL (High-P Sieverts system)

Kinetics

Intematix (Combinatorial – mainly catalysts; nanoparticle synthesis)
Utah (Catalysts)
Hawaii (Novel catalysts)

"The synergy, made possible by the Center, between materials discovery and fundamental studies, is critical to eventual success"

-- Zak Fang, U of Utah (Proj. C POC)

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Working Together in Project D

Regeneration

BNL/ORNL (amide-alane mixtures)
SRNL (Electrochemical)
Hawaii (supercritical fluid approaches)

System Studies

BNL (Synthesis and kinetics)
SRNL (Proto-type tank studies)
SNL (Engineering properties)

Advanced Characterization

BNL (Synchrotron XRD, DSC, TEM, TPD)
JPL (NMR)
Hawaii/NIST (Neutron scattering)

Theory

MHCoE Theory Group
(first principle amine-alane models)

Theory-Expt. Collaboration:
BNL needs guidance on stabilities of alane-Lewis Acid complexes

i.e., TEDA + Al* + H_2 ↔ TEDA-AlH_3
(Triethylenediamine)

Theory Group: Calculate gas-phase complex stabilities to guide BNL regeneration efforts

"The MHCoE approach covers all aspects of alane research from fundamental theory to tank design and testing."

-- Jim Wegrzyn, BNL (Project D POC)

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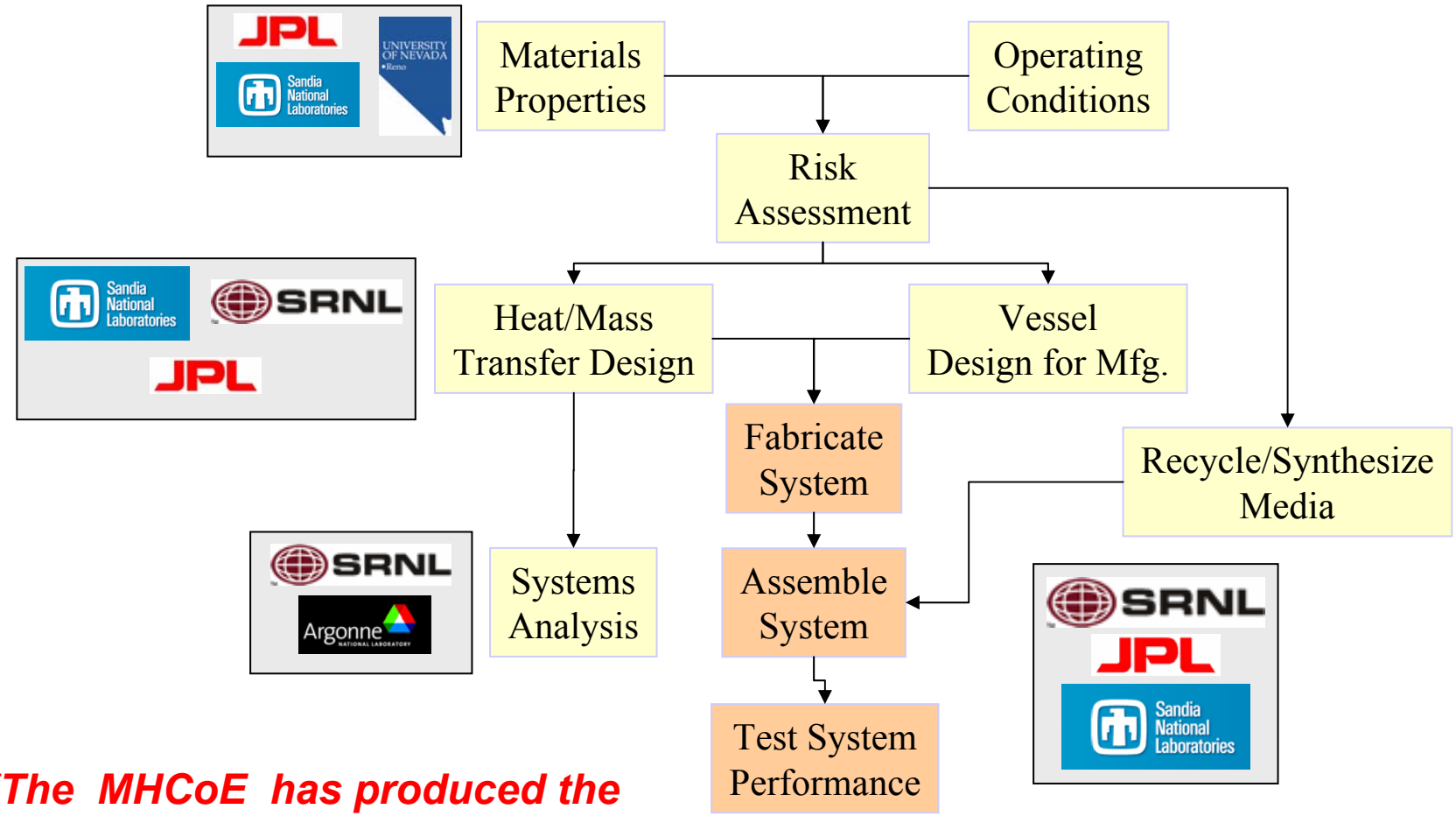
Working Together in Project E



"The MHCoE has produced the collaboration, at a level of interaction not previously achieved, of a broadly-experienced team of hydrogen storage engineering experts"

--Don Anton, SRNL (Proj. E POC)

MHCoE Contacts with Other Groups

MHCoE/Carbon Center:

MHCoE Coordinating Council tours the Carbon Center on 7/18/2006, meets PI's, discusses Carbon Center work

MHCoE/Chemical Center:

Initial meeting on 5/17/2007 to initiate contacts, discuss Al regeneration (Proj. D)

MHCoE/Berkeley H_2 Storage Group:

Two meetings on 7/21/06, 3/13/07 at LBNL

Examined nano approaches to improving kinetics, thermodynamics in AlH_3, destabilized systems

-- Agreed we should cooperate in developing metal hydride nanoparticle superlattices--

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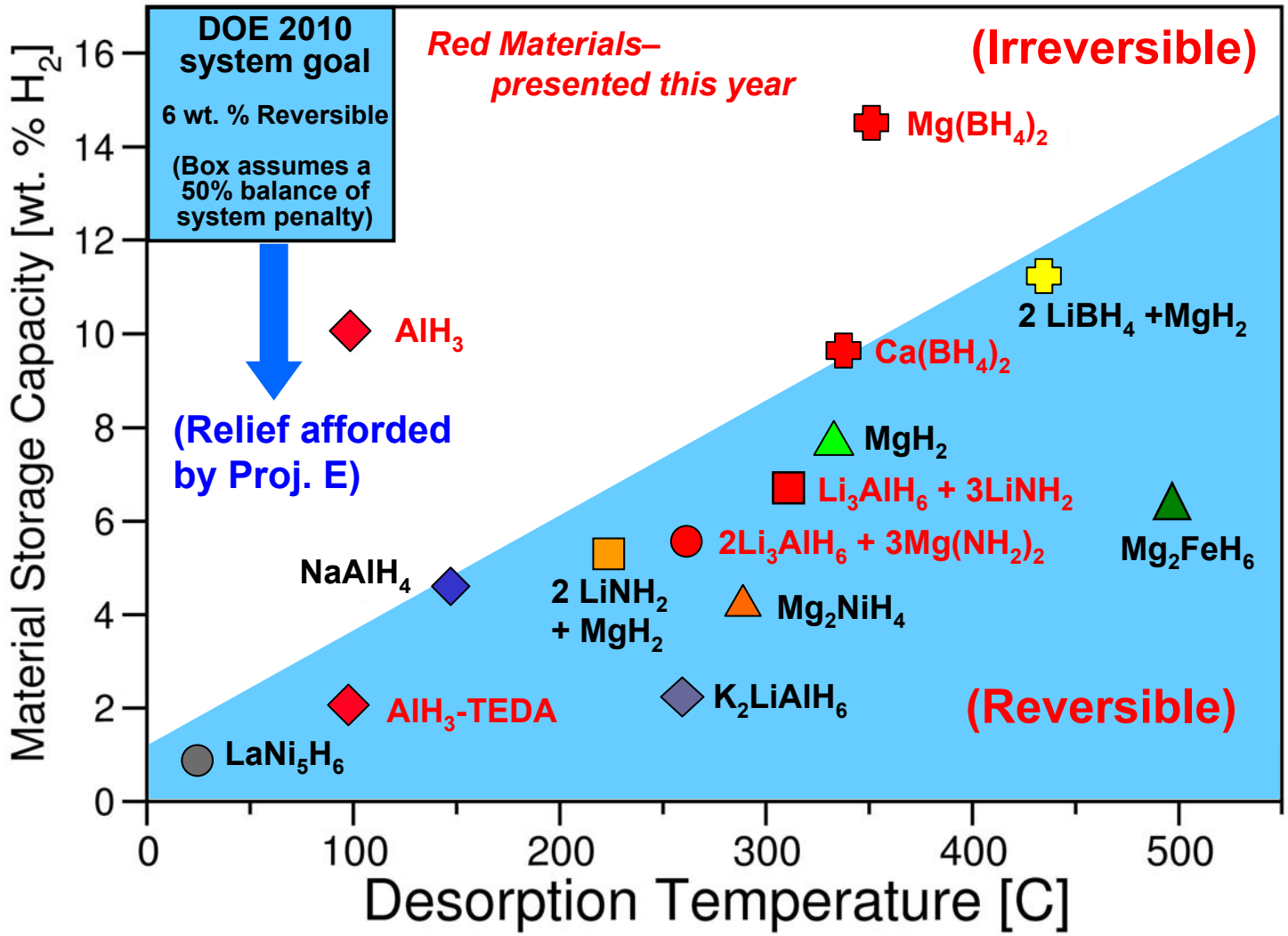
MHCoE Materials Relative to DOE Targets



(Original plot from GE)

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Closing the Gaps

The MHCoE collaborations are focussed on closing the gaps between the materials' performance and the DOE 2010 goals….

Weight Capacity: **Emphasizing high wt. % systems:**

2007 Project B– $Mg(BH_4)_2$, $Ca(BH_4)_2$

2007 Project E– reduced system penalty

Reversibility: **Exploring effects of additives on reversibility:**

2007 Project B– $Ca(BH_4)_2$ reversible with additive

Thermodynamics: **Investigating destabilization, nanoconfinement:**

2007 Project A– Sc predicted to lower ΔH for $LiBH_4$

Kinetics: **Exploring additives, nanoconfinement to improve kinetics:**

2007 Project C– $LiNH_2$ lowers the E_a for $LiAlH_4$, Li_3AlH_6 to release hydrogen

Combinatorial studies will be important in the materials discovery, guided by theory

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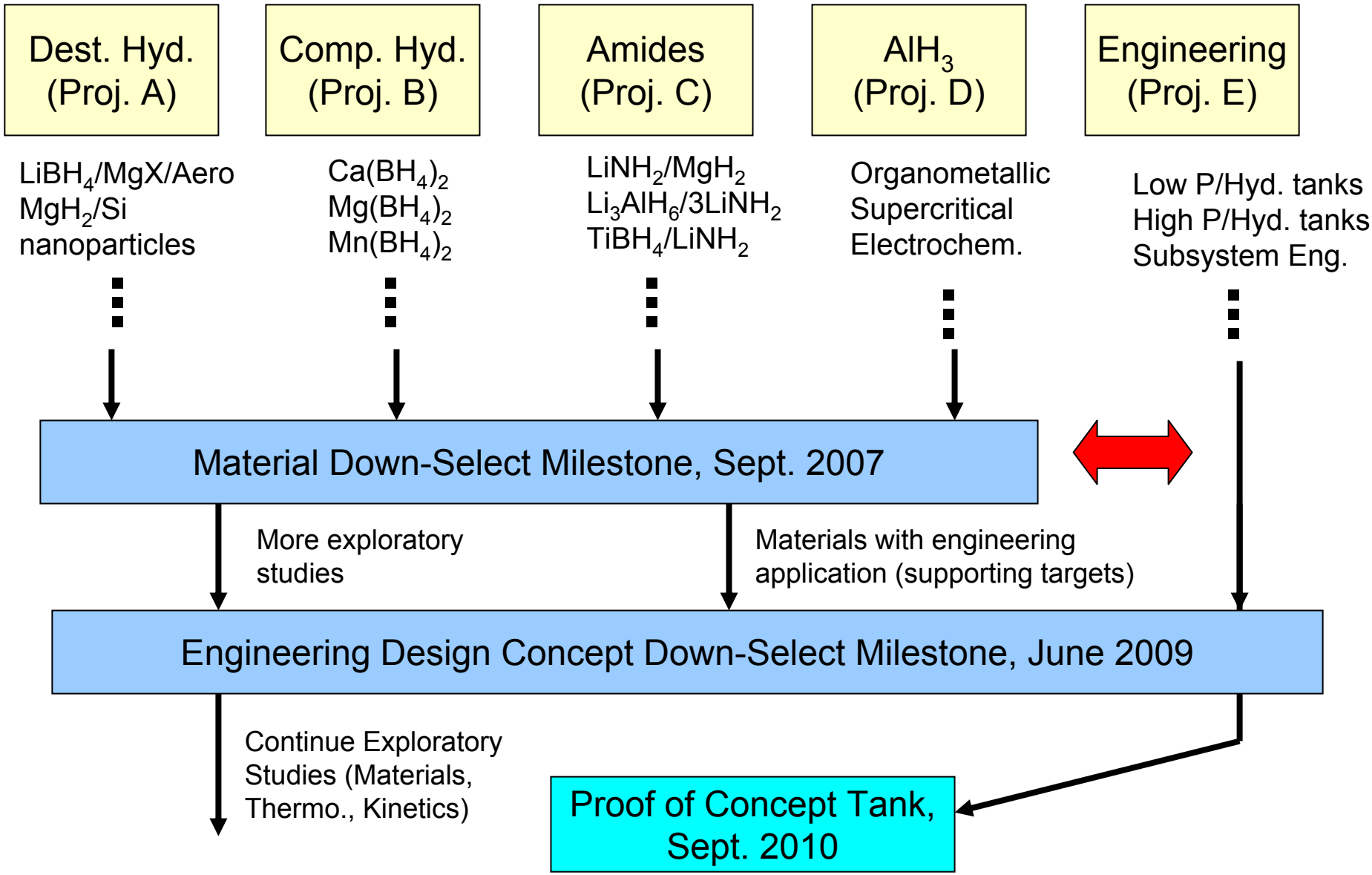
Overall Direction of the MHCoE



MHCoE Meeting, Livermore CA, October 30, 2006