Metal Hydride Center of Excellence



Lennie Klebanoff, Director Jay Keller, Deputy Director

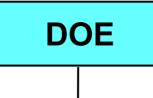
Project ID# STP 11

This presentation does not contain any proprietary information



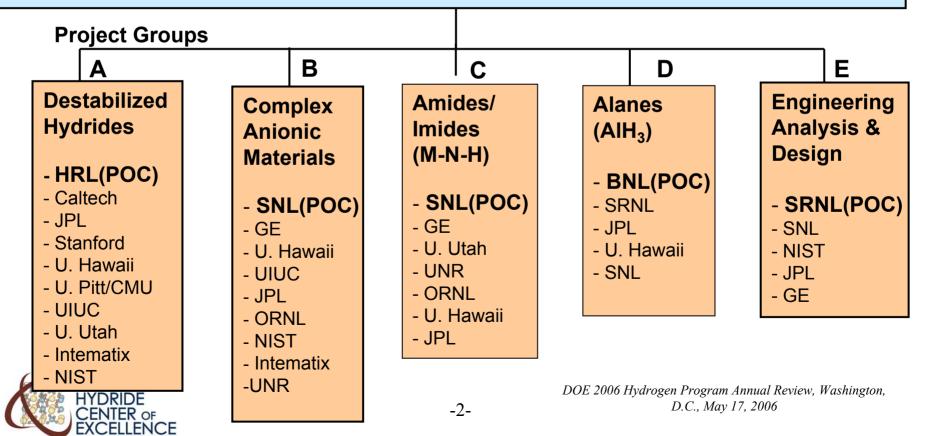
DOE 2006 Hydrogen Program Annual Review, Washington, D.C., May 17, 2006

New MHCoE Project Structure



Coordinating Council (2006)

Greg Olson (HRL), Craig Jensen (UH), Lennie Klebanoff (SNL), Jay Keller (SNL) Jim Wegrzyn (BNL), Ian Robertson (UIUC), Bruce Clemens (Stanford)



Project A – Destabilized Hydrides

Develop strategies for reducing H₂ storage thermal requirements, improve kinetics

Technical Approaches:

Alter Thermodynamics by Hydride Destabilization:

> Reduce energy needed to liberate H_2 by forming dehydrogenated alloy, thereby reducing desorption temperature.

Enhance Kinetics by Nanoengineering:

Minimize required H diffusion distance by using scaffolds, decreasing particle size

See talk by: Greg Olson, HRL



Project B - Complex Anionic Materials

Predict, synthesize and evaluate promising new complex hydride materials

Technical Approach:

- Develop efficient Monte Carlo method to assess energetics of starting compounds, intermediate species, and end products.
- Guided by theory, discover candidate metal hydrides by highhydrogen pressure sintering, measure hydrogen sorption properties
- Work initially with a known compound to develop strategy (K₂LiAlH₆)



Project C - Amides/Imides

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

Technical Approach:

- Reduce thermal requirements of amides by alloying
- Examine chemical pathways, side reactions, new synthetic routes
- Determine initial engineering issues (thermal cycling, expansion)



Project D - Alane (AlH₃)

Objective: Understand desorption and regeneration properties of alane for H₂ storage

 α -AIH₃ \longrightarrow AI + 3/2 H₂ H-capacity (g) = 10.1 wt%

Technical Approach:

- > Examine prospects for regeneration from AI + H_2
- Synthesize AIH₃ polymorphs
- Evaluate thermodynamic/kinetic properties of different alane phases
- Measure crystallographic structure of different phases

See talk by: Jason Graetz, BNL

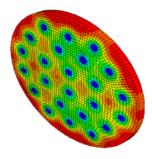


Project E - Engineering Analysis, Design & Test

Objective: Provide engineering, analysis and design supporting DOE system performance goals

Technical Approach:

- > Develop engineering system-level storage models
- > Use engineering models to provide targeted materials properties
- Perform thermal modeling of candidate hydride materials
- Conduct expansion, stress measurements of promising materials
- Determine heat transfer properties of new hydrides



Thermal Modeling

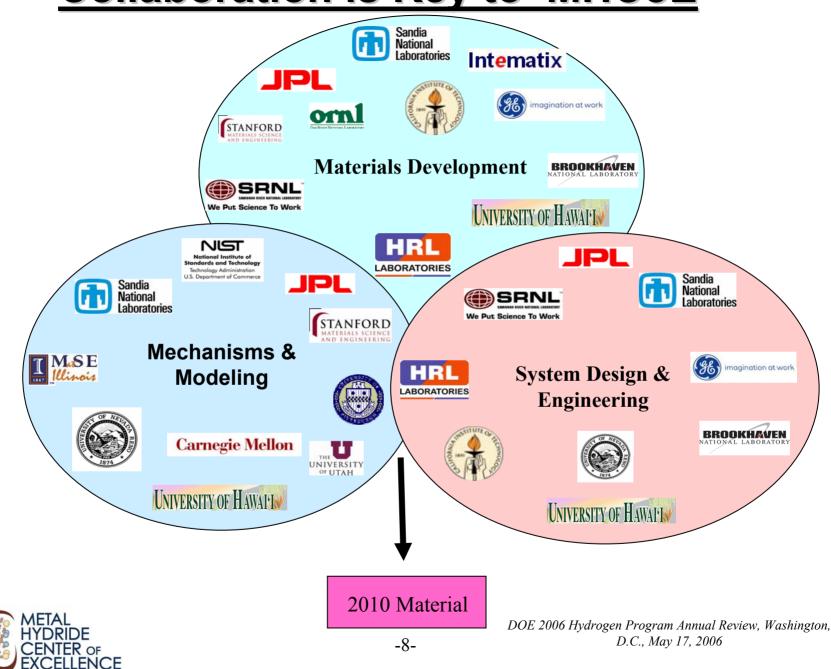




See poster by: SRNL

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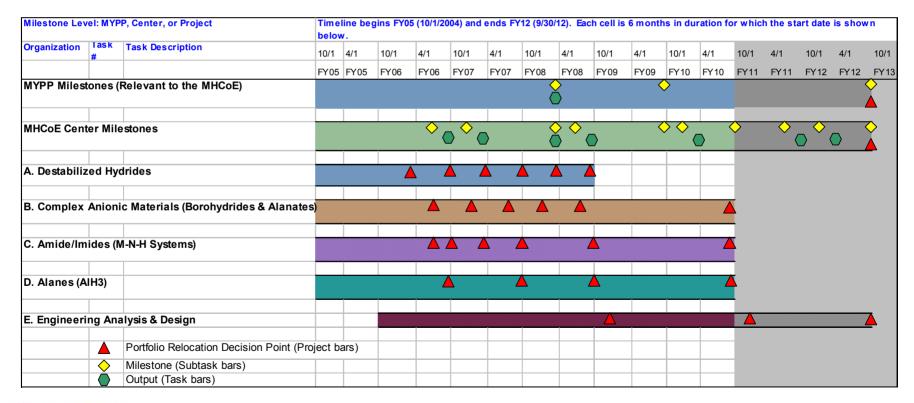
Collaboration is Key to MHCoE



Project Groups Milestone Chart

Milestone Chart has been implemented Center-wide:

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





Greater Detail Available for Projects A-E

Milestone L	.evel: MY	PP, Center, or Project	Timeline below.	e be	gins FY0	5 (10/1/2	004) and	ends F	(12 (9/30	/12). Eac	ch cell is	6 month	ns in du	ration f	or whic	h the st	art date	is show	wn
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	#		FY05 F		FY06	FY 06	FY07	FY07	FY08	FY08	FY 09	FY 09	FY10	FY10	FY11			FY12	
MYPP Milestones (Relevant to the MHCoE)			1100 11	00	1100	1100	1101	1107	(1105	<	>	1110			1112	1112	
MHCoE Center Milestones						`)		$\left \right\rangle $		· <	$> \diamond \langle$		\diamond	¢,		\bigcirc	$\mathbf{\hat{A}}$
A. Destabi	lized Hy	ydrides			/		<u> </u>	<u> </u>	<u> </u>		\								
B. Comple	ex Anior	nic Materials (Borohydrides & Alanates)			Á									Z				
C. Amide/	lmides ((M-N-H Systems)				Á	Á 4	<u> </u>											
D. Alanes	(AIH3)					4	4	-	4		A				2				
E. Enginee	ering Ar	nalysis & Design									À				À				7
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SNL/JPL	1.2	Materials Compatibility					<	\diamond			<	\diamond				\diamond			
JPL	1.3	Vessel Testing (Detailed Component						<pre> </pre>	\diamond			<hr/>	>				\diamond		
	2	Media Engineering Development										($\overline{\mathbf{O}}$		
	3	Safety Strategies						(<u> </u>				\bigcirc				Ō		
	4	Prototype Vessels									\bigcirc				\bigcirc				$\overline{\mathbf{O}}$
	5	System Modeling										ï	-		0				$\overline{\mathbf{O}}$
		Portfolio Relocation Decision Point (Pro	ject bars)															
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	Ó	Output (Task bars)																	

