2007 DOE Chemical Hydrogen Storage Center of Excellence Overview

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Los Alamos National Laboratory

May 17, 2007

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Overview

Timeline

- Start date: Jan - April 2005
- End date: Jan. 2010
- Completion: Approx. 40%

Barriers Addressed

- Hydrogen release capacities
- Hydrogen release rates
- Regeneration of spent fuel
- Regeneration efficiency

Budget

- FY07 -- 50/300K PNNL/LANL: Center Coordination Funding

Partners: 2 NLs, 7 Universities, 4 Companies

LANL, PNNL; U. Alabama, UC Davis, U. Missouri, Northern Arizona U., U. Penn, Penn State U., U. Washington, U. S. Borax (Rio Tinto), Intematix, Millennium Cell, Rohm and Haas

Objectives

Identify, research, develop and validate advanced on-board chemical hydrogen storage systems to overcome technical barriers and meet 2010 DOE system goals with the potential to meet 2015 goals:

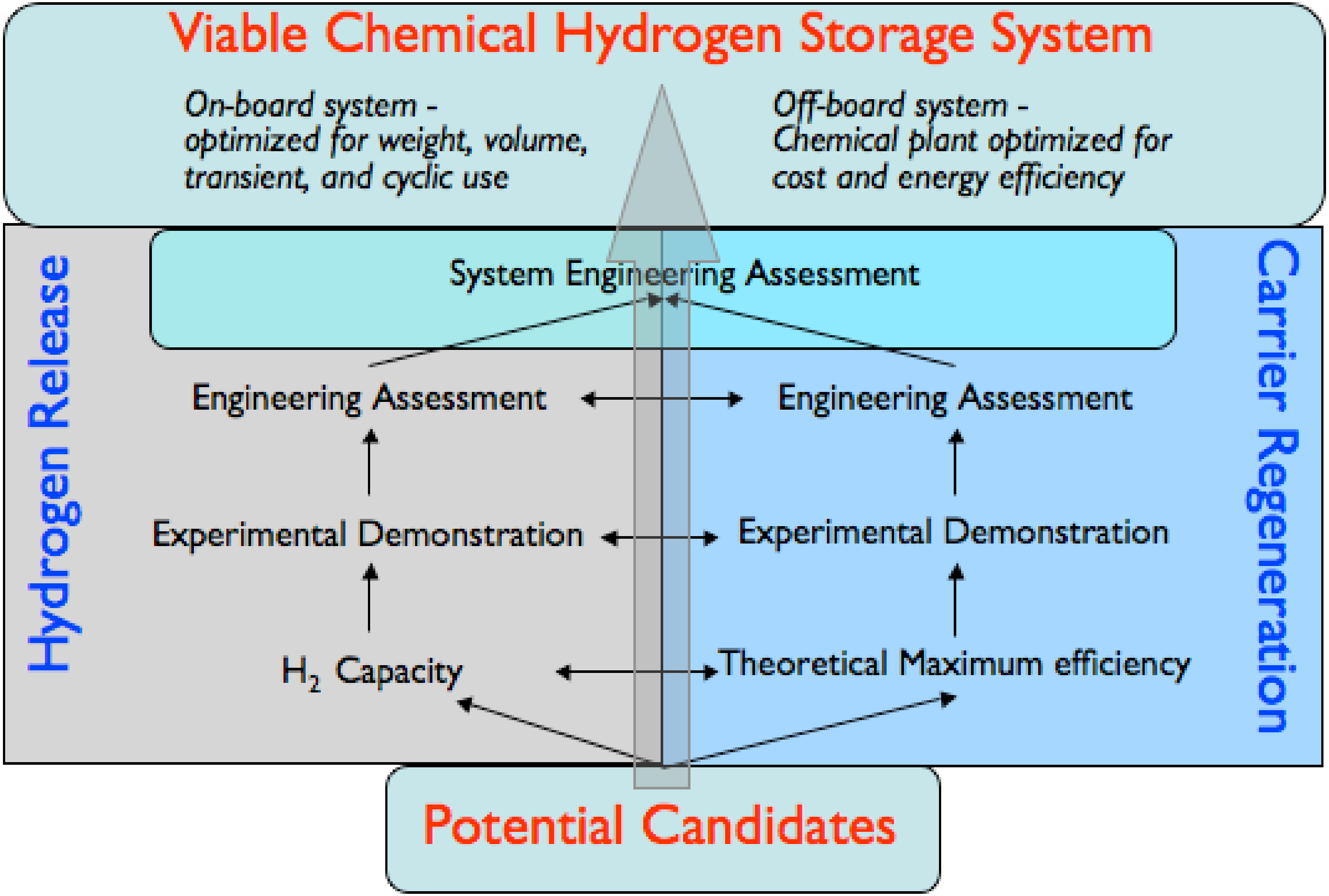
- Develop materials, catalysts and new concepts to control thermochemistry and reaction pathways
- Assess concepts and systems using engineering analysis and studies
- Select most promising chemical systems for engineering development
- Develop life cycle inventory and demonstrate a 1 kg storage system

Approach to Technical Barriers

- CAPACITY
  - Develop, synthesize, test compounds with high hydrogen density, favorable energetics, and potential pathways
  - Theory and modeling for insight to materials discovery and optimization
- HYDROGEN RELEASE
  - Develop materials and pathways that avoid large thermodynamic sinks and non-productive byproducts
  - Study mechanisms to enhance rates, extents of release, and to aid in the design of catalysts
  - Develop and optimize catalysts and catalytic processes
- REGENERATION
  - Develop pathways close to thermodynamic limits
    - Avoid high energy intermediates
    - Use recyclable intermediates
- ENGINEERING ANALYSIS
  - Provide early assessment of viability
  - Develop viable candidates toward prototype

Theory ⟷ Experiment ⟷ Assessment

Performance-Based Approach



Overview of Current Center Activities

- Tier I Sodium Borohydride
  - Regeneration Pathways Assessment
  - Electrochemical Reduction
  - On-board Engineering Assessment

R&H, PSU, LANL, PNNL, Ala, MCEL

- Tier II: Alternative Boron Chemistries
  - Amine Borane (AB/MeAB) Dehydrogenation
    - Mechanisms
    - Modifiers; chemical additives
    - Liquid fuel compositions
    - Catalyst development
  - AB Regeneration
    - Digestion of spent fuel, followed by
    - Reduction and ammoniation back to AB
    - Integration of all process steps
  - Polyhedralborane hydrolysis

Penn, NAU, Ala, Washington, LANL, PNNL, Missouri, Intematix, Davis

- Tier III: Advanced Concepts
  - Organic systems
  - Nanomaterials
  - Coupled reactions
  - Metal amine boranes (with International Partnership for the Hydrogen Economy, IPHE -- new collaboration)

Ala, Davis, LANL, PNNL

Center Capabilities

Capability	U. Ala.	UCD	U. MIssou	N. Ariz. U.	U. Penn	PSU	U. Wash.	Intematix	MCEL	R&H	PNNL	LANL
Synthesis	x	x	x	x	x		x	x			x	x
Rapid Screening								x			x	x
Characterization	x	x	x	x	x		x	x		x	x	x
Electrochemistry						x						
Hydrogen Release	x	x	x		x		x	x	x		x	x
Regen Chemistry		x			x					x	x	x
Theory	x				x							
Catalyst Synthesis							x	x			x	x
Catalysis							x	x			x	x
Eng. Assess.									x	x	x	x
Reaction Eng.									x	x	x	x
Process Design									x	x	x	x
Prototyping									x	x		

Center Integrates Capabilities to Enhance Progress

Tier I
BO to BH

Engineering Assessment
Theory and Modeling
Reactor Modeling
Electrochemistry
Regeneration Chemistry
Process Design

R&H, PSU, LANL, PNNL, Ala, MCEL

Tier II
Alternative Boron Chem.

Materials Synthesis
Characterization
Theory and Modeling
Regeneration Chemistry
Rapid Screening
Hydrogen Release
Catalyst Synthesis
Catalysis
Engineering Assessment

Penn, NAU, Ala, Washington, LANL, PNNL, Missouri, Intematix, Davis

Tier III
Advanced Concepts

Materials Synthesis
Characterization
Theory and Modeling
Regeneration Chemistry
Rapid Screening
Hydrogen Release
Catalyst Synthesis
Catalysis

Ala, Davis, LANL, PNNL

Theory and Modeling Crosscut Center Efforts for Early Assessment and to Guide Experiment

- Tier I Sodium Borohydride
  - Hydride reduction energetics (Rohm and Haas)
  - On-board reactor modeling (PNNL, MCEL)
- Tier II Alternative Boron Chemistries
  - Calculation of energetics of dehydrogenation reactions and reaction intermediates (Alabama, LANL, PNNL)
  - NMR chemical shift prediction in support of experiment (Penn, Alabama, LANL)
  - Thermochemistry of AB spent fuel regeneration: digestion, disproportionation, hydride transfer (Alabama, PNNL, LANL, Penn, UC Davis)
- Tier III Advanced Concepts
  - Calculation of Si-H vs. B-H bond energies to predict energetics of nanoparticle chemistries (Alabama, UC Davis)
  - Heats of formation and reaction enthalpies for heteroatom organics (Alabama, Washington)
  - Thermochemistry of IPHE project materials (Alabama, LANL, PNNL)

Engineering Assessment & Coordination Crosscuts Center Activities (PNNL Lead)

- Analysis: Rohm & Haas (lead), Millennium Cell, PNNL, LANL
- Fuel Stability: PNNL (lead), Rohm & Haas, NAU
- Hydrolysis Systems: Millennium Cell (lead), PNNL
- New Process Concepts: PNNL, LANL, Rohm & Haas, Millennium Cell
- AB Regeneration: LANL, Rohm & Haas, PNNL
- Catalysis requirements: LANL, PNNL

Coordination between engineering and scientific advances critical to Center success

ROHM AND HAAS
Pacific Northwest National Laboratory
Operated by Battelle for the U.S. Department of Energy
Millennium Cell
NORTHERN ARIZONA UNIVERSITY
Los Alamos NATIONAL LABORATORY EST. 1943

Key Milestones
and technical barriers to be addressed

- DOE's SBH Go/No-Go decision 4QFY07
- Near-term regeneration:
  - Achieve near-quantitative mass balance for regeneration
  - Achieve > 60% thermodynamic efficiency with optimized recycle chemistry
- Near-term AB H_2 release:
  - Catalysis: achieve >2 equiv. H_2 at higher rates
  - Thermolysis: Demonstrate solid AB reactor and process
- Down-select 2-3 materials and processes within the Center for engineering and development studies to meet 2010 targets (1QFY08)
- Down-select materials for further research to meet 2015 targets (1QFY08)
- Demonstrate chemical hydrogen regeneration laboratory-scale process for 2010 targets and for materials with potential to meet 2015 targets

SBH Go/No-Go Milestones: FY07

Q1	Finish computational analysis of Sodium Borohydride (SBH) regeneration options (chemical and electrolytic) that meet regeneration efficiency criteria (efficiency target of 50%)** and identify at least one process for laboratory demonstration. (quarterly report from Rohm and Haas)
Q2	Complete conceptual on-board system design that includes a path forward to meet the 2010 targets for on-board gravimetric and volumetric density. (quarterly report from Millennium Cell/PNNL)
Q3	Determine if laboratory demonstration of all non-commercial or unproven SBH formation steps are possible and estimate the efficiency** of the overall process. Prepare preliminary SBH production/regeneration cost estimate that contains a sensitivity analysis and qualifies the estimate in terms of degree of confidence (quarterly report from PSU, PNNL, ROH, LANL).
Q4	Determine feasibility and provide a go/no-go recommendation for SBH hydrolysis on-board storage system based on modeling of on-board storage system and laboratory-scale experimental demonstration of energy efficient** regeneration off-board. (recommendation from Center Coordinating Council)

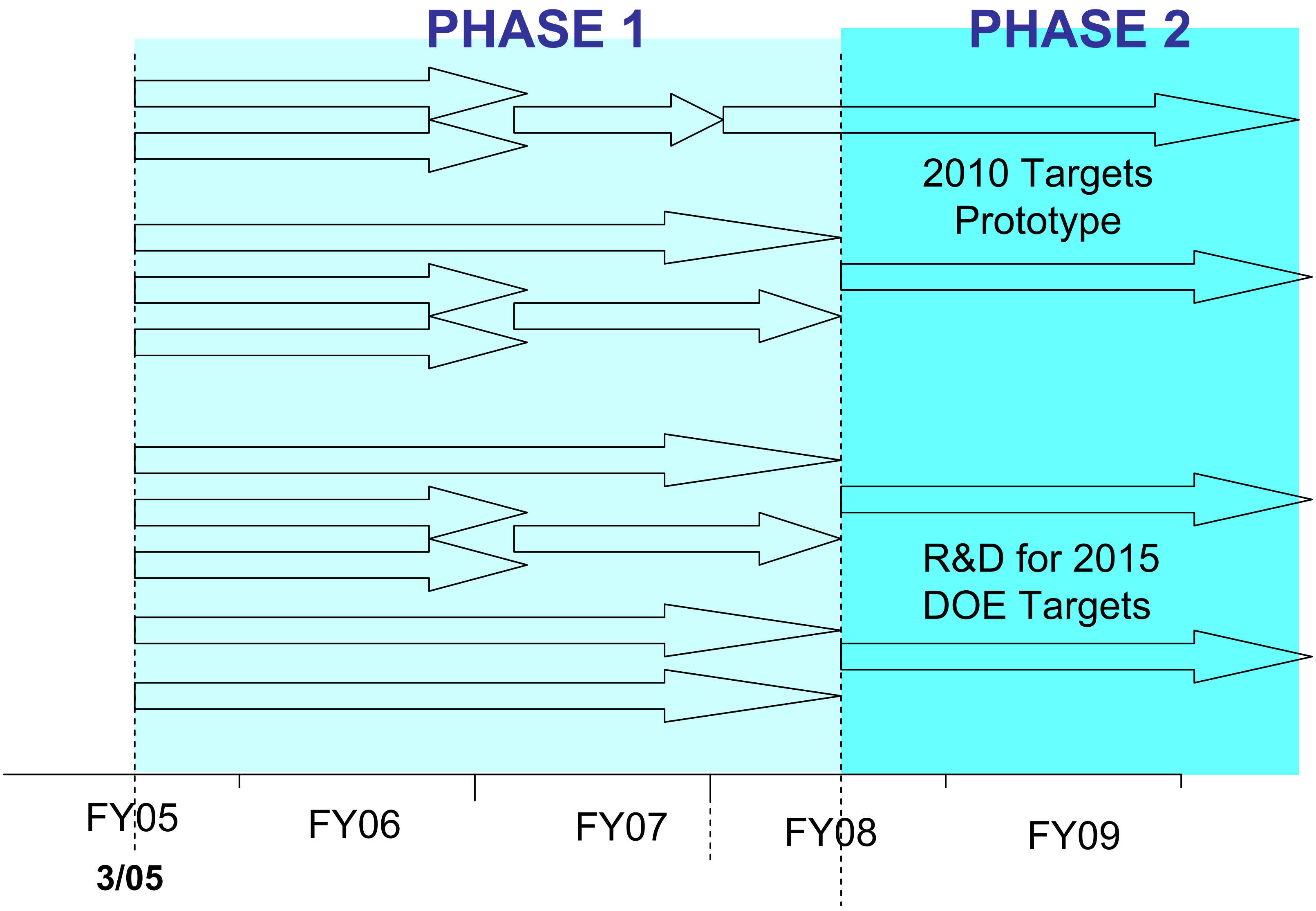
DOE's Independent Review Panel scheduled to convene early September

Materials Down Select Process

DOE 2010 Target	Metric	Material 1	Material 2	Material n
System gravimetric Capacity (6 wt %)	g hydrogen released/g lab vessel	✓	✓	✓
System Volumetric Capacity (.045 kg/L)	kg hydrogen/L lab vessel	✓	?	✓
H_2 Flow rate (0.02 g/s/kW (80 kW stack)	ml lab reactor to achieve .8 mole H_2/sec	✓	✓	no
Regen Efficiency > 60 %	Based on LHV H_2, regen thermodynamics, demonstrated chemistry	✓	?	--
Auxiliary physical and chemical properties metrics	Solids, liquids, slurries, reactivity, handling, stability, byproducts, safety, etc.		?	

Materials down selections (current and to Phase 2) are based on progress (tracked quarterly) toward meeting DOE Targets

Phase 1 to Phase 2 Transition



Phase 1 to 2 Down Selection Process : Partner Capabilities Mapped to Down Selected Materials

Partner Capabilities	Material 1	Material 2	Material n
Materials synthesis and characterization			
Catalysis and catalyst synthesis			
Kinetics and Mechanism			
Theory and Modeling			
Reaction engineering			
Process modeling			
Systems integration			
…			

Partners

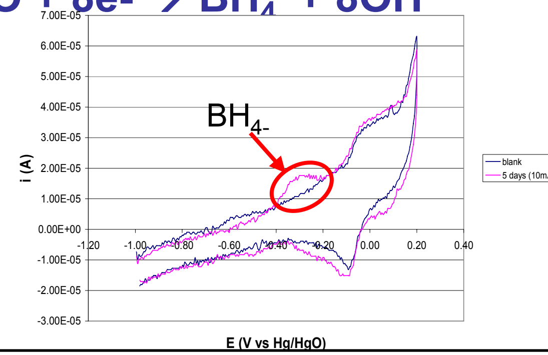
Continued partner participation in Phase 2 will be determined within Center and based on capabilities required to achieve Phase 2 goals on down selected materials

Tier I: Technical Accomplishments

- Regeneration of BO to BH pathways assessed and proof-of-principle demonstrated
- Engineering assessment of SBH hydrogen release delivered
- Go/No-Go milestones developed with DOE

- Electrochemistry
  - PSU demonstrates proof-of-principle borate reduction

$$B(OH)_4^- + 4H_2O + 8e^- \rightarrow BH_4^- + 8OH^-$$



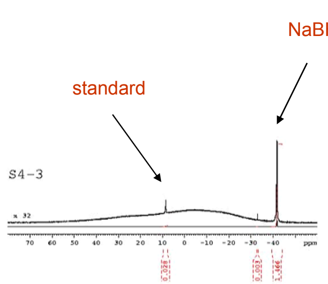
PENNSTATE

ROHM AND HAAS

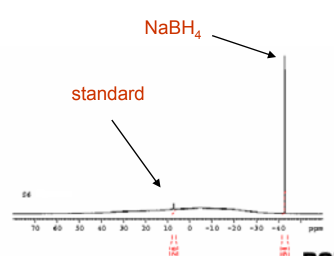
- Metal reduction
  - R&H demonstrates proof-of-principle borate reduction

$$NaBO_2 + 2x/y\ M + 2H_2 \rightarrow NaBH_4 + 2/y\ MxOy$$

Metal Hydride A



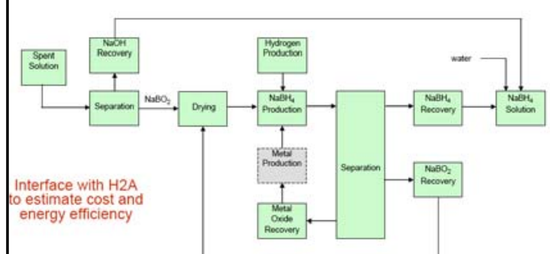
Metal Hydride C

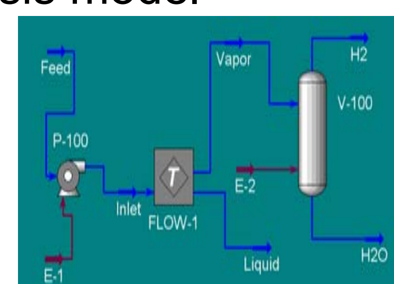


ROHM AND HAAS

Engineering assessment:

- MCEL preliminary design package delivered
- R&H assessed regeneration pathways
- Implemented H2A analysis model





ROHM AND HAAS

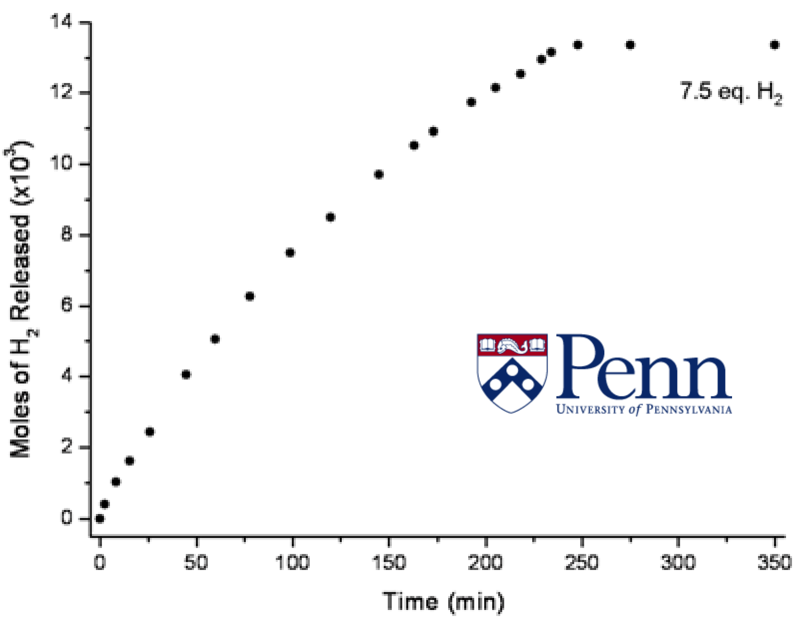
Pacific Northwest National Laboratory

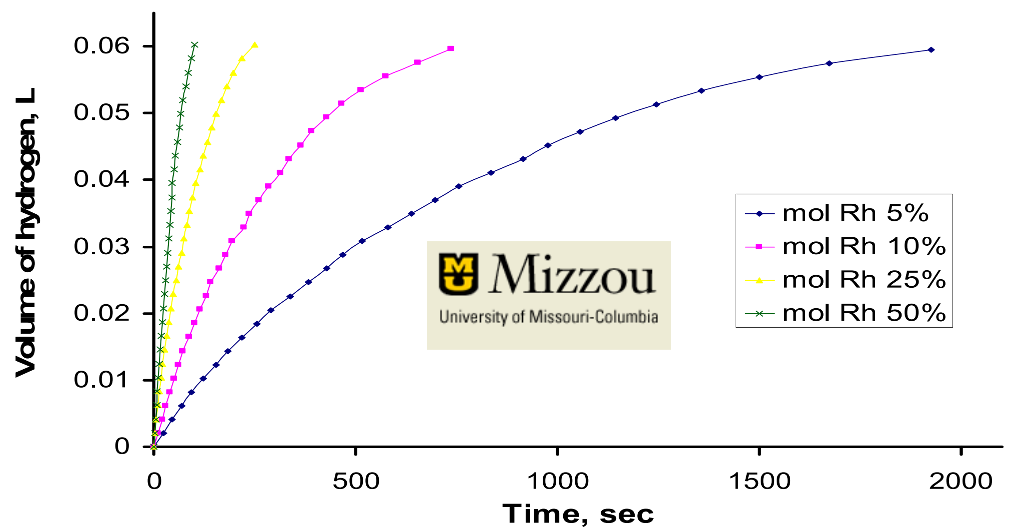
Millennium Cell

Key Results
Tier II: Complex Boranes

- Hydrolysis of ammonia triborane (AT) ($NH_3B_3H_7 + 6H_2O$)
  - Rh catalysed hydrolysis releases 6.1 wt. % H_2
  - 2010 and 2015 system targets not attainable with AT hydrolysis
  - Completed AT hydrolysis work at Penn

- Hydrolysis of $K_2B_{10}H_{10}$+32 H_2O
  - Rh catalysed hydrolysis releases 5.6 wt. % H_2
  - pH and counter ions for polyhedral borane anions have little effect on rate, extent of H_2
  - Go/No-Go tied to SBH decision





DOE System Targets: 2007, 4.5 wt%**; 2010,** 6.0 wt%; **2015**, 9.0 wt%

Tier II: Alternative Boron Materials

Because of their protonic N-H and hydridic B-H hydrogens, amineboranes, ABs, are unique in their ability to store and release hydrogen while avoiding B-O formation

$$\overset{\delta^{-}H\quad H^{\delta+}}{\text{AB: } H_2B\text{-}NH_2} \longrightarrow \text{--}HB\text{-}NH\text{--} + H_2$$

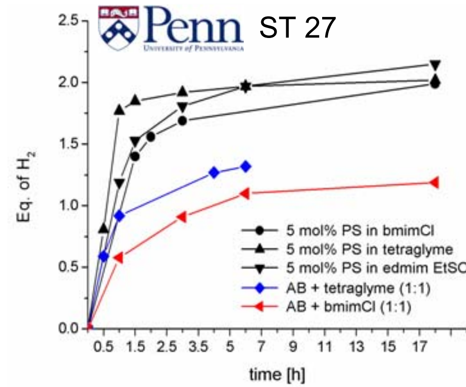
$$\text{AB: } H_3B\text{-}NH_3 \xrightarrow{-H_2} \text{cyclotriborazane} \xrightarrow{-H_2} \text{Borazine} \xrightarrow{-H_2} \text{Polyborazylene} \xrightarrow{-H_2} \text{'BN''}$$

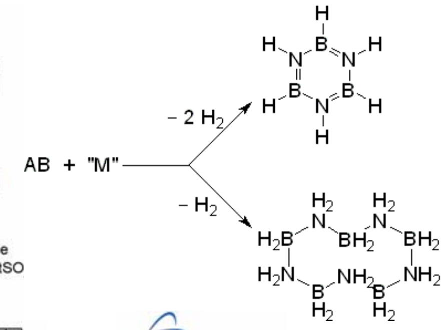
	H_2 wt%, H_2 density (assumes conv. to 'BN')	properties
NH_4BH_4	24.5%, 0.2 kg-H_2/L;	Unstable > -20°C
AB: NH_3BH_3	19.6, 0.16	Crystalline solid
Cyclotriborazane: $B_3N_3H_{12}$	14.9, 0.11	Crystalline solid
Borazine: $B_3N_3H_6$	7.5, 0.06	Liquid, bp 55 °C
AT: $NH_3B_3H_7$	17.8, 0.14	Crystalline solid
MeAB: $BH_3NH_2CH_3$	8.9, 0.08 (assuming 2H_2/MeAB)	Solid, mp 55 °C

DOE System Targets: **2007** 4.5 wt %, 0.036 kg-H_2/L; **2010**: 6.0 wt. %, 0.045 kg-H_2/L; **2015**: 9.0 wt%, 0.081 kg-H_2/L

Tier II: Selected Results from Hydrogen Release from Amine Boranes

- Mechanistic understanding has led to increased capacities and rates
  - –Penn: Anionic mechanism in ionic liquids
  - –LANL: Metal catalyzed mechanisms explain selectivity, capacities, and guide catalyst design
- Understanding of chemistry and engineering issues has led to new liquid amine borane formulations
  - –PNNL and LANL provide proof-of-principle for RNH_2BH_3
  - –NAU discovers liquid formulation of MeAB/AB
  - –U. Washington demonstrates high rates of H_2 release
- Solid AB: >16 wt % release (PNNL)
- Large parameter space requires rapid throughput screening
  - – LANL - new rapid throughput for homogeneous catalysts for H_2 release
  - – Intematix - Solid catalysts for H_2 release
  - – Future -- Regeneration





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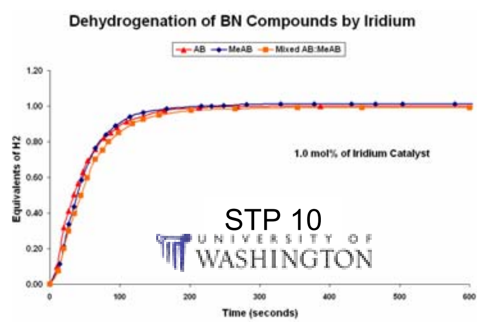
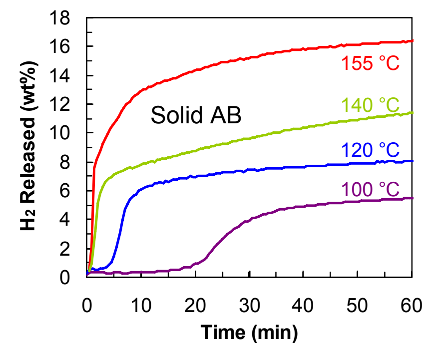
NORTHERN ARIZONA UNIVERSITY STP 8 THE UNIVERSITY OF ALABAMA ST 30





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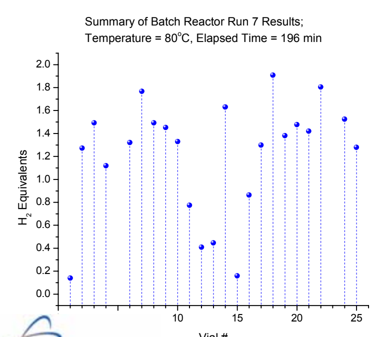

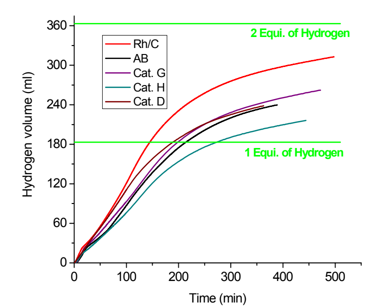

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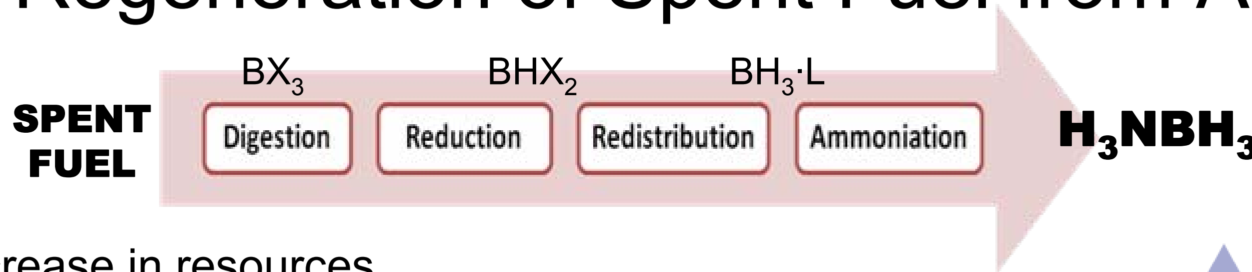
Intematix STP 13

Key Results: AB Hydrogen Release

- Thermolysis/Chemical Promoters
  - Anionic polymerization mechanism enhances extent, rates of release
  - Ionic liquids avoid induction period, promote reactivity, improve rates and extent of release from AB
  - Chemical promoters alter reaction pathway, enhance extent of release
- Solid AB Thermolysis
  - Mechanistic understanding of release from solid AB
  - Chemical additives reduce induction period, alter ‘nucleation and growth’ phase
  - Demonstrated up to 16 wt. % H_2
  - Fuel stability studies ongoing
- Metal Catalysis
  - Improved mechanistic understanding drives catalyst design
  - Equally rapid release of 1 H_2 from AB and MeAB with Ir catalysts at room temperature
  - Greater extent of H_2 with inexpensive base metal catalysts at improved rates at T > 60 °C (patents)
  - Liquid fuel compositions: MeAB/AB
  - MeAB/AB release rates and capacities improving with better catalysts
  - MeAB dehydrogenation (-1H_2) results in soluble spent fuel products
- Completed Bronsted acid-catalysed release from AB at LANL

Tier II: Regeneration of Spent Fuel from ABs



- Significant increase in resources directed at regeneration chemistry
- Regeneration of spent fuel demonstrated by two pathways
  - Spent fuel ⟶ BBr_3 ⟶ AB
  - Spent fuel ⟶ BSR_n ⟶ AB
  - Capture of residual B-H
  - Theory input guided experiments

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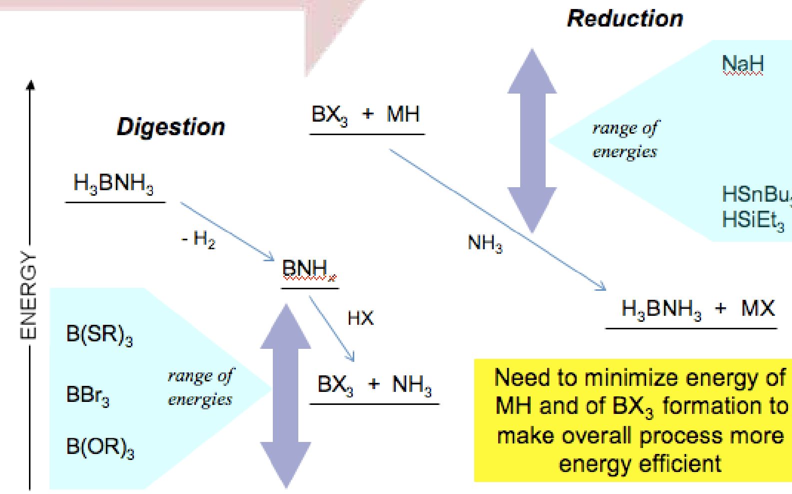
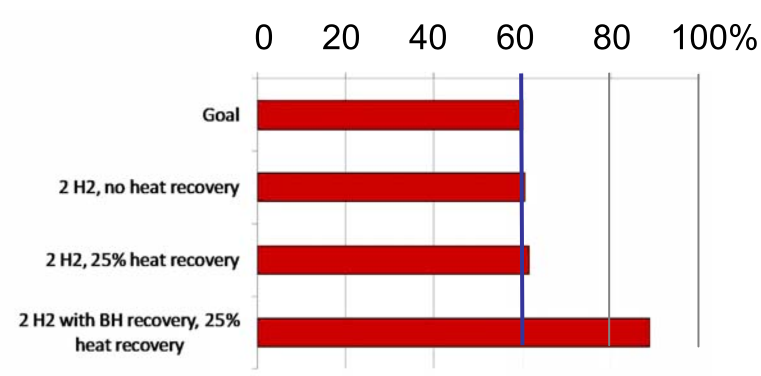
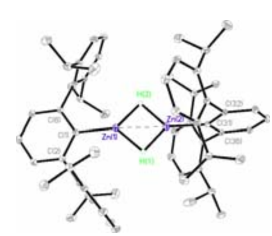


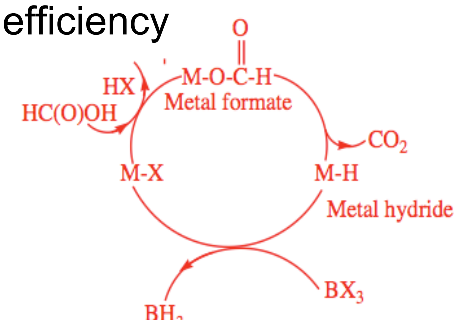
- Overall regeneration efficiencies calculated, e.g. spent fuel-BSR_n-SnH-AB:



- Recycle of reducing agents
  - UC Davis and Alabama working on M-X to M-H recycle and energetics
  - Crucial to overall efficiency



Structure of a new Zn-H for M-H recycle



STP 14

Key Results: Spent Fuel Regeneration

Placed substantially more resources on regeneration this year

- FY06 Status: proof-of-principle chemistry studies initiated
  - Penn demonstrated trifluoroacetic acid digestion
  - Penn demonstrated amine AlH_3 reduction to amine borane
  - LANL demonstrated Sn-H reduction of Cl-BCat to make HBCat; subsequent disproportionation to BH_3 (patent)
  - LANL: possible recycle of Sn-Cl to Sn-H with formate (patent)
- FY07 Status - *all steps of two potential regen chemistries demonstrated and efficiencies calculated*
  - Penn: Br approach
  - LANL: SR approach (patent app. pending)
  - UC Davis: exploring M-X to M-H recycle
- Routes to 'save' B-H in spent fuel
  - PNNL: strained alkoxides to $(RO)_2B$-H, ammonia digestion
  - LANL: spent B-H to $(RS)_2B$-H; +NH_3(liq.) directly to AB

Tier I&II: Materials Comparisons and Progress Selected Results

Metrics	Hydrolysis			Thermolysis/Chemical Promoters				
	Penn AT (1.1 mol % Rh)	MCEL 30 wt% aq. SBH	Missouri $K_2B_{10}H_{10}$ Rh	PNNL AB solid 120 °C 140 °C	PNNL AB solid 155 °C (avg. rate to n H_2)	Penn AB/$LiNH_2$, 85 °C, 3 hr	Penn AB/AT/PS, solid state 85 °C, 3 hr	Penn AB/AT/PS, ionic liquid, 85 °C, 3 hr
Grav. density (Mat. wt%)	6.1, 4h	Material 7.3% System 4.5%	5.6	7 >13	>16	5.9	6.9	6.5
Vol. density (kg-H_2/L	0.090, 4h	System .037	.083	.021 .039	.048	.047	0.059	0.060
H_2 Flow Rate (g/s) per kg	0.0042, 4h	System 0.024	-	1 (max rate) 1.8 (max)	.84 (1 H_2) .22 (2^+ H_2)	.0055	0.0064	.0060
Kg of Mat. for 0.8 mol/s	377, 4h (halted work)	-	1.8	2 (max) 1 (max rate)	0.8 (max rate)	295	250	267

DOE System Targets for Hydrogen Storage Systems

Gravimetric Density (wt%)
4.5 ***(2007)***, 6.0 ***(2010)***, 9.0 ***(2015)***

Volumetric Density (Kg-H_2/L)
0.036 ***(2007)***, 0.045 ***(2010)***, 0.081 ***(2015)***

Tier II: Materials Comparisons and Progress Selected Results

Metrics	Catalysis						
	UW Ir, AB w/solvent, 23 °C	LANL Ni, MeAB/AB (neat) 80 °C	1: 1 MeAB/AB Theoretical, 2 equivalents H_2	LANL Ni cat 2% AB, in solvent 80 °C	Extrapolated Ni AB, saturated sol'n	LANL Ru cat, 2% AB in solvent 80 °C	LANL Bronsted Acid; 20 wt % AB, 60 °C 18 hr
Grav. density (Mat. wt%)	0.4 (4.9 - no solvent)	5.7	11	.015 10.8 - no solvent	1.8	0.019 13.5 - ns	1.7
Vol. density (Kg-H_2/L Mat.)	0.005	0.06	0.12	0.00015 .08 - ns	.03	.00019 .1 - ns	0.016
H_2 Flow Rate (g/s) per kg Mat.	0.068 0.82 - ns	0.02	-	0.00002 .016 - ns	.004	0.0001 .01 - ns	18 hrs -- too slow
Kg of Mat. for 0.8 mol/s	24 2 - ns	100	-	70,000 98 - ns	400	16,000 160 - ns	work halted

[ns -- no solvent included in calculation]

DOE System Targets for Hydrogen Storage Systems

Gravimetric Density (wt%)
4.5 ***(2007)***, 6.0 ***(2010)***, 9.0 ***(2015)***

Volumetric Density (Kg-H_2/L)
0.036 ***(2007)***, 0.045 ***(2010)***, 0.081 ***(2015)***

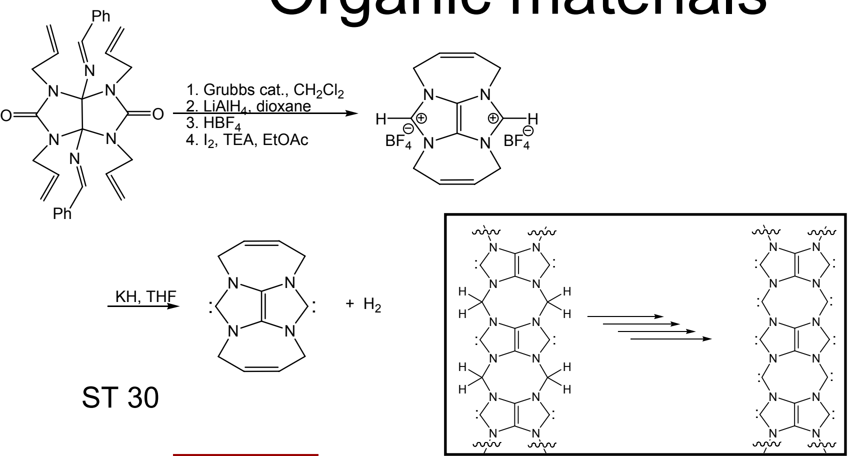
Tier III: Advanced Concepts

- Organics - contain appreciable hydrogen for release
  - Demonstrated 1,1-elimination of hydrogen to make carbene
    - Currently 2 wt% of possible 7.2 wt%
  - Demonstrated hydrolysis of carbenes
  - 1,5-Elimination to diimidazolium rings
- Nanoparticles
  - UC Davis demonstrated hydrogen release from Si nanoparticles (TG/MS); not reversible
  - Terminated nanoparticle work at LANL
- Coupled Reactions
  - Goal is to develop concepts with > 1 H/carbon or hetero atom
  - Developed 25 well reactor for catalyst screening and hydrogen quantification (Center capability)
- IPHE - new start Winter, 06
  - Metal amine boranes - potential up to 11.9 wt % H_2; reversible?
  - Patent application

IPHE International Partnership for the Hydrogen Economy | The University of Alabama | University of California Davis | Intematix | Los Alamos National Laboratory EST. 1943 | Pacific Northwest National Laboratory Operated by Battelle for the U.S. Department of Energy

Tier III Advanced Concepts

Organic materials



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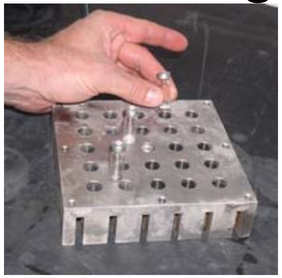
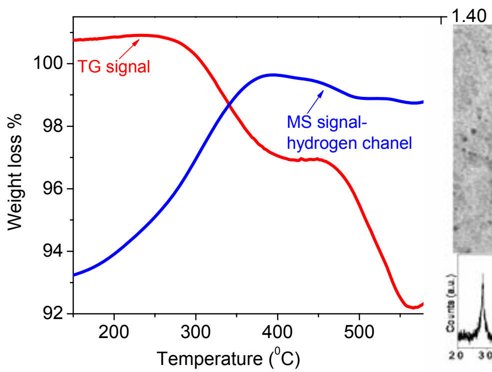
Prepared precursor to 7.2% polymer

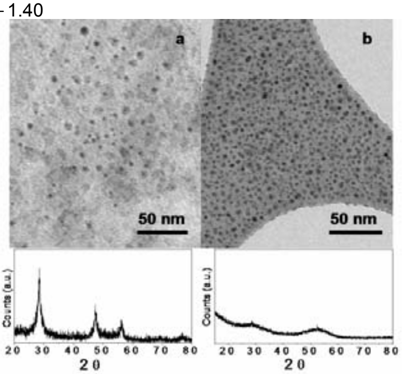
Rapid Throughput



- Two 25-well plate batch reactors fabricated
- H_2 quantification by gas chromatography

Nanomaterials





TG/MS showing ~3 wt % H_2 between 200-350˚C.

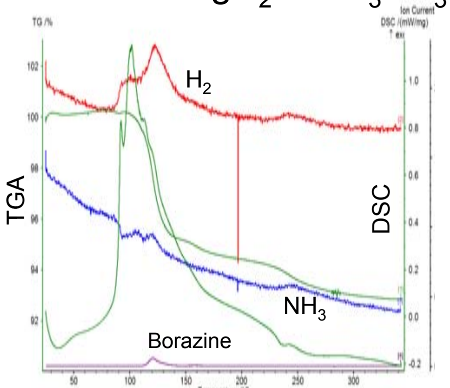
~5 nm diameter Si nanoparticles

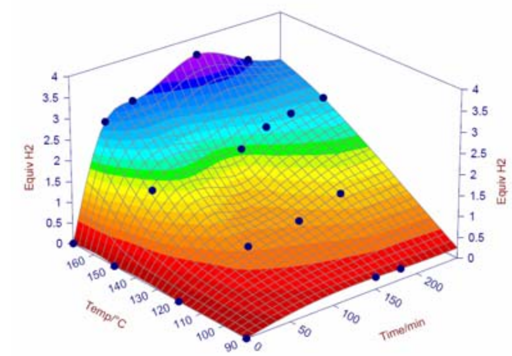
STP 14

IPHE materials

ST 28, -29

Ball milled MgH_2 + NH_3BH_3





7.2 % H_2 quantified by GC

Tier III: Materials Comparisons and Progress
Selected Results

Metrics	Tier III Advanced Concepts				
	Organic Hydrides Theory	Coupled Reactions Theory	IPHE Theory	Nano Theory	Washington /Alabama BNHC's Theory
Grav. density (Mat. wt%)	[0.9 -- 2006[a]] 2[b] 7.2	[4.4- 2006] -[c] 8-9	Measured 7.2 Max 10 - 11.9 Opt. 8-10.9	4.5[d] 8-11	- 7-8%
Vol. density (Kg-H_2/L Mat.)	['06-- .015]] 0.045	0.04	Measured 0.072	.1	tbd
H_2 Flow Rate (g/s) per kg Mat.	tbd	.008	Measured 0.02	tbd	tbd
Kg of Mat. for 0.8 mol/sec	tbd	195	Measured 80	tbd	tbd

a. benzimidizole, terminated; b. U. Alabama carbenes proposed;
c. 2007 work focused on IPHE, rapid screening; d. preliminary results on 4 nm particles

DOE System Targets for Hydrogen Storage Systems

Gravimetric Density (wt%)
4.5 ***(2007)***, 6.0 ***(2010)***, 9.0 ***(2015)***

Volumetric Density (Kg-H_2/L)
0.036 ***(2007)***, 0.045 ***(2010)***, 0.081 ***(2015)***

Engineering Assessment & Coordination (PNNL, Lead)

- Analysis: Rohm & Haas (lead), Millennium Cell, PNNL, LANL
- Fuel Stability: PNNL (lead), Rohm & Haas, NAU
- Hydrolysis Systems: Millennium Cell (lead), PNNL
- New Process Concepts: PNNL, LANL, Rohm & Haas, Millennium Cell
- AB Regeneration: LANL, Rohm & Haas, PNNL
- Catalysis: LANL, PNNL

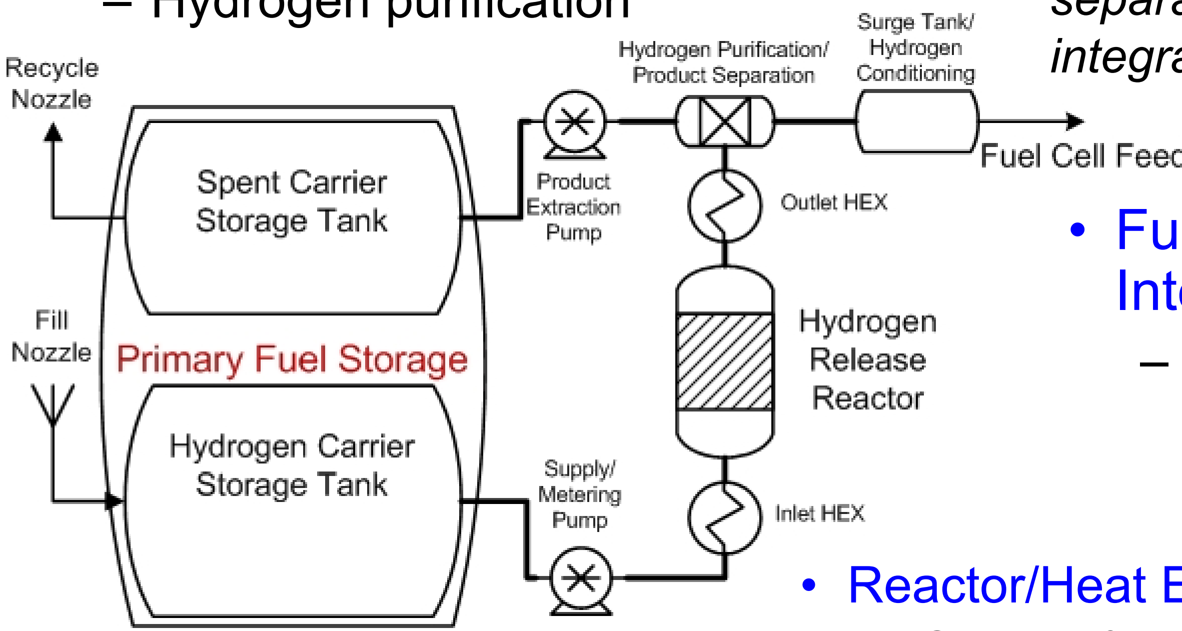
Coordination between engineering and scientific advances critical to Center success

ROHM AND HAAS
Pacific Northwest National Laboratory
Operated by Battelle for the U.S. Department of Energy
Millennium Cell
NORTHERN ARIZONA UNIVERSITY
Los Alamos NATIONAL LABORATORY EST. 1943

Functional Schematic of an Onboard Storage System - Engineering Research Needs

- Products of Hydrogen Release:
  - Separation requirements
  - Hydrogen purification

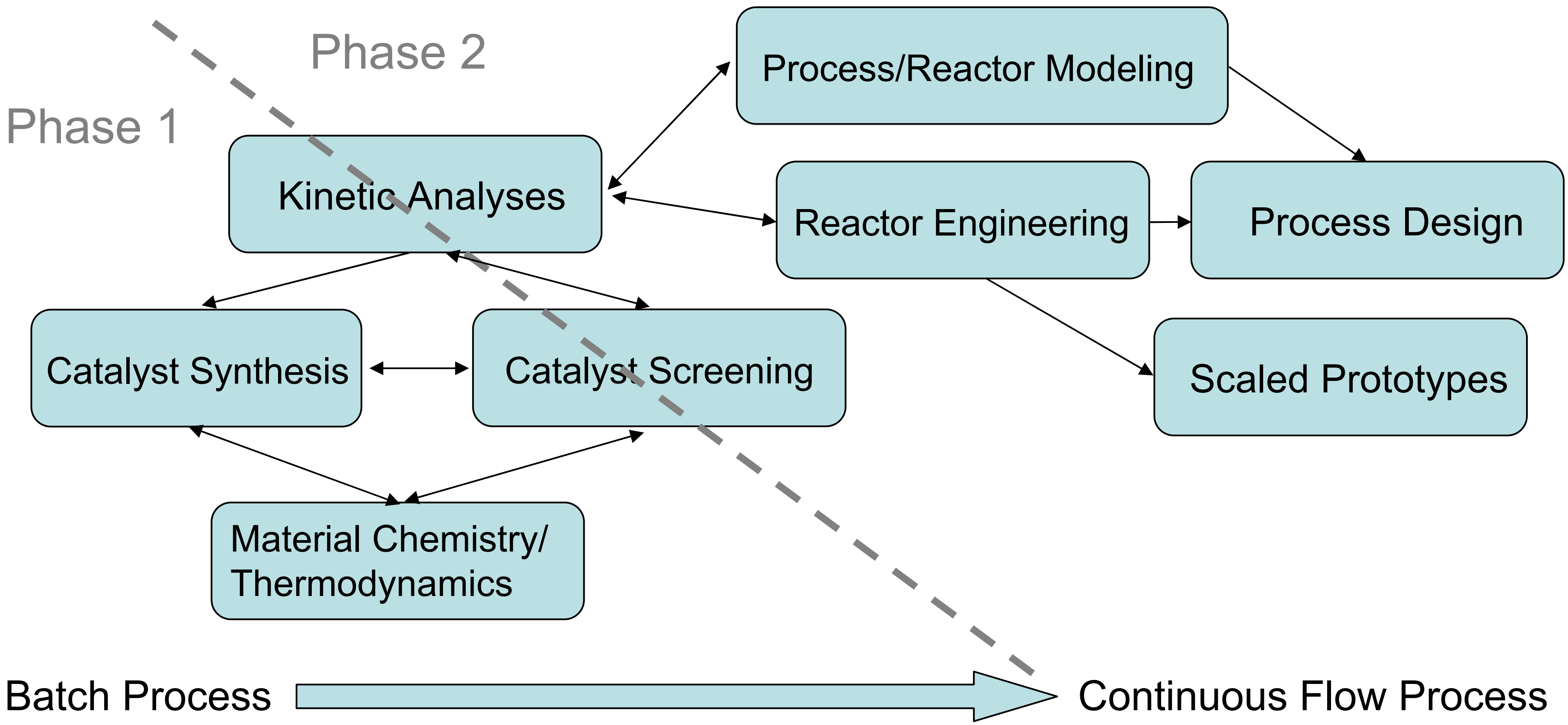
Components identified separately, but could be integrated



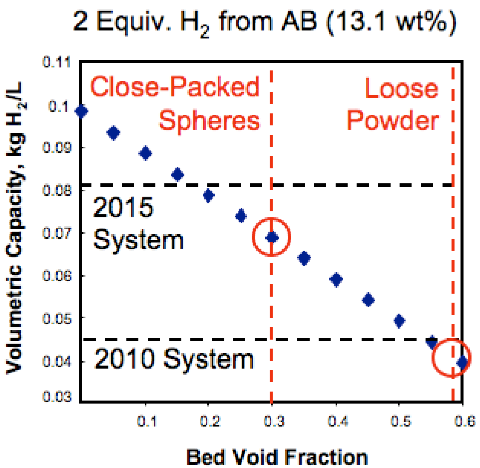
- Fuel Cell System Integration:
  - Match Hydrogen flow to fuel cell requirements over the drive cycle
- Reactor/Heat Exchange:
  - Catalyst & structure
  - Catalyst kinetics
  - Heat exchange requirements & thermal integration with the fuel cell
- Fuel Storage:
  - Fuel formulation
  - Fuel stability
  - Storage geometry for volumetric capacity

Engineering Approach

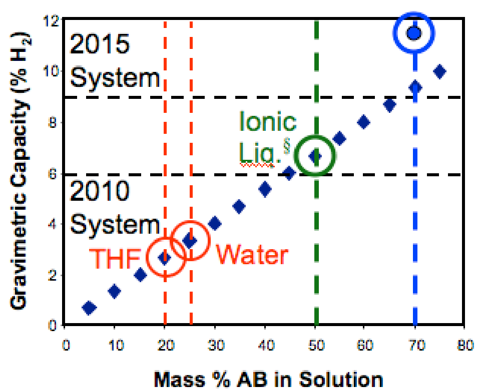
Developing the tools - modeling, experimental apparatus, and experiments - to move from batch processes to continuous flow processes



Engineering Assessment Tier II/III: Key Results

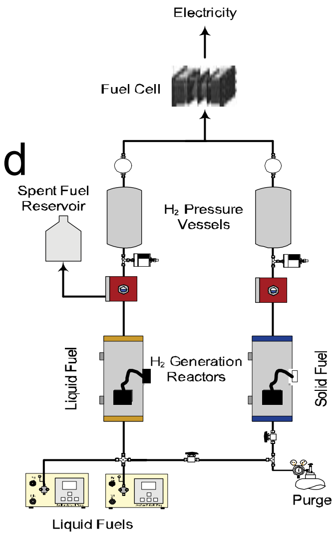


- Bed void volume limits capacity to achieve goals



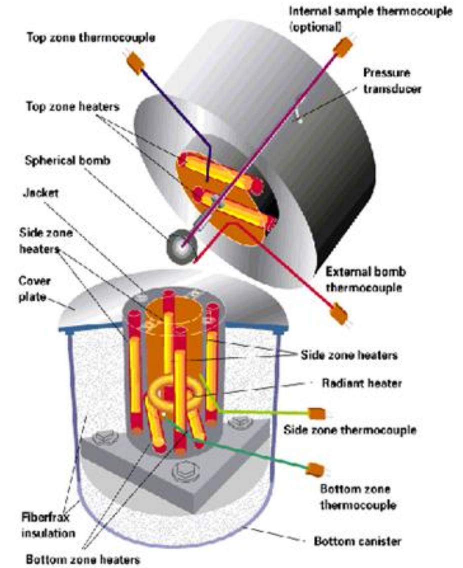
- Solvents limit capacity to achieve goals

- 'Breadboard' approach to rapid prototyping for continuous processing



Hydrogen Release

- Accelerated rate calorimeter used to define solid AB fuel stability from number of vendors



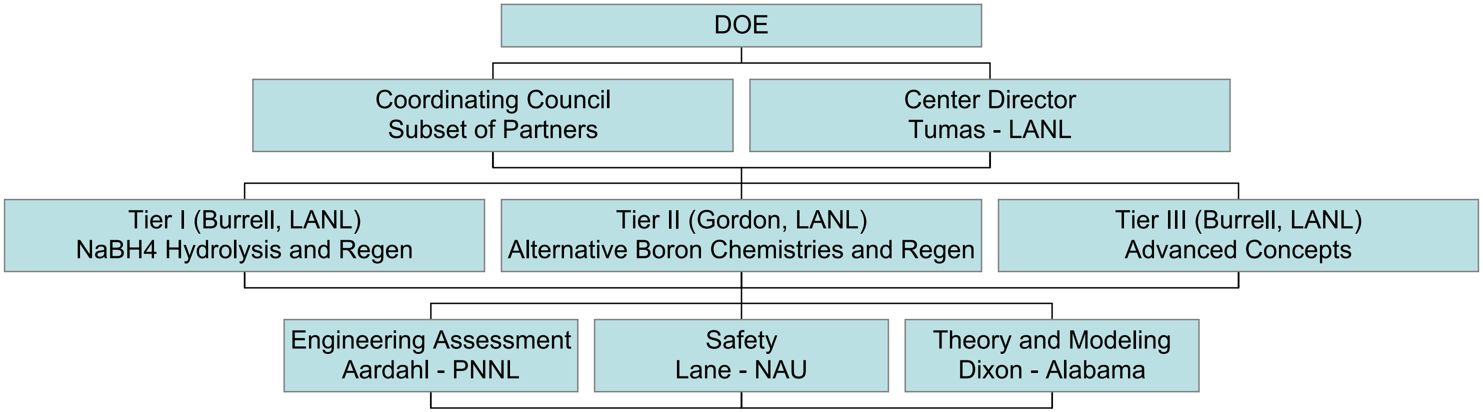
Summary

- Engineering analysis and regeneration pathway selection completed for SBH and Go/No-Go milestones developed
- Polyhedralboranes hydrolysis tied to SBH Go/No-Go
- Demonstrated potential of liquid fuel amine boranes; high capacity release from solid AB, high rate catalysts and high capacity catalysts for amine borane H_2 release
- Demonstrated two distinct regeneration chemistries of spent fuel AB, efficiencies calculated approaching or exceeding the target
- Theory and modeling continue to play an integral role in guiding and interpreting experiments
- New solid materials being developed with promising preliminary results
- New heteroatom-substituted organics and hybrid organic amine boranes being developed
- Engineering assessments guiding experiments; leading toward down selection criteria and prototype processes

Future Work

- Continue to innovate and to develop many promising materials and regeneration options to maintain a ‘pipeline’ of candidates
  - High capacity materials with high rates of H_2 release
  - ≥ 2 H released / element; AB = 2^+; more candidates needed
  - Innovate on release from organics ≥ 2H/C
  - Search for materials regenerable with H_2
  - Hybrid materials - e.g. IPHE project
- Improve efficiency of existing AB regeneration schemes
  - Novel digestion agents
  - Improved, efficient recycle of hydride transfer agents
  - Continue to search for liquid fuel compositions
  - Enhance rates, extent of release through catalyst design
- Continue to use quarterly reporting matrix to guide offramp decisions; re-direct resources where needed
- Engineering - move from batch to continuous processes

Center Management and Communication

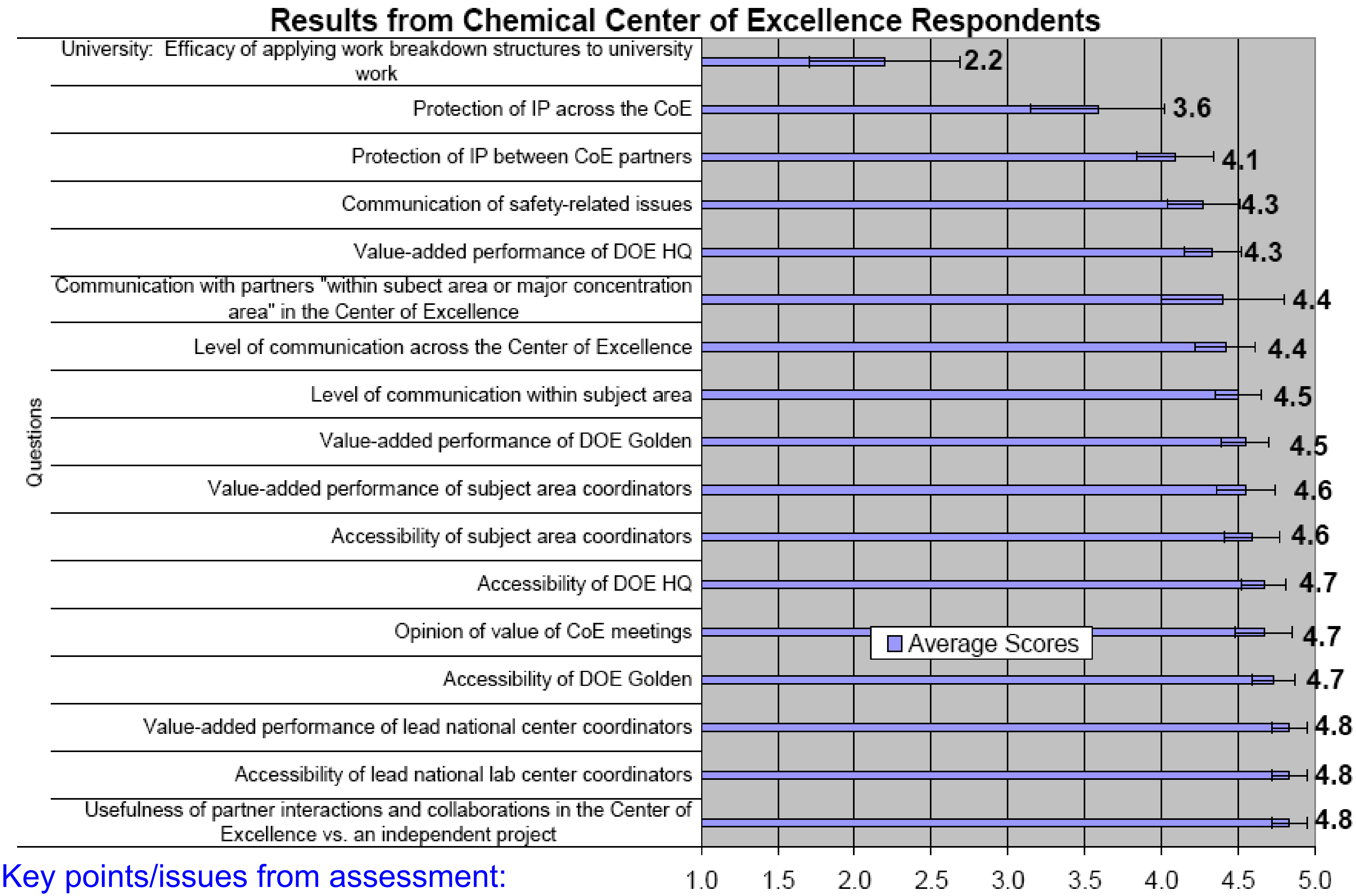


- Established IP agreement that allows free exchange of ideas and materials among Center partners
- Tiers are coordinated through single LANL point of contact; Coordinating Council (slide 40)
- Projects within Tiers have single POCs, e.g. AB regen, BO to BH e-chem, etc.
- Regular tier and sub-tier conference calls and meetings, frequent one-on-one phone calls, site visits to exchange information in real time
  – eg. AB regen meeting, electrochem conf. calls, IPHE meetings, integration of theory/modeling, engineering conference call, etc.
- Quarterly tracking of Partner’s progress toward DOE target capacities, rates, regeneration efficiencies, etc.
- Develop materials down selection criteria and recommends down selection, revision of workscope decisions with Coordinating Council input; input to Phase 1 to 2 transition
- Hydrogen Storage Centers conference calls with DOE to foster cross-Center information exchange with Carbon- and Metal Hydride Storage Centers
- Biannual Center meetings coincident with Tech Team and Annual Review
- Participation in Storage Systems Analysis Working Group: cross-Center engineering issues
- Organize Annual Review, Tech Team Review

Key Impacts of Center Communications

- Mid-year Center Coordination meeting (Denver)
  - ID Center Capabilities and Gaps
    - Re-directed Center resources to regeneration: UC Davis chemistry expertise to work on M-X to M-H recycle
    - Brought more focus to Engineering Assessment, added LANL expertise to the team
  - Developed Center-wide quarterly reporting matrix for chemical hydrogen storage materials (release capacity, rates, conditions, etc.)
  - Identified gap in Center capability - rapid throughput for homogeneous H_2 release catalysts
- Tier and Subtier Conference calls
  - E-chem conf. call -- LANL assists Penn State e-chem effort with synthetic chemistry support
  - Coordinated NAUs MeAB/AB work to rapidly get samples to other partners for testing
  - Decision to suspend LANL Bronsted acid-catalysed AB H_2 release, LANL nanoparticle work
  - SBH Go/No-Go milestones developed via Tier I meetings, conference calls
  - Tied polyhedral boranes materials down selection to SBH Go/No-Go
  - Tier II/III Center-wide equipment needs -- developed Center prioritization for DOE
  - Sharing of samples for further characterization
  - Feedback mechanisms to increase rate of progress, Center-wide
- Coordinate personnel exchange
  - Bowden (IRL) to PNNL&LANL; LANL staff to Oxford (collaborations with IPHE)
  - Grad students use of equipment for data collection at National Labs

Self Assessment



- Key points/issues from assessment:
  - Milestone driven research and academic cultures
  - IP procedures across complex Center structure still improving
  - Communication across Center/DOE is very good
  - Integrated Center adds value vs. independent projects