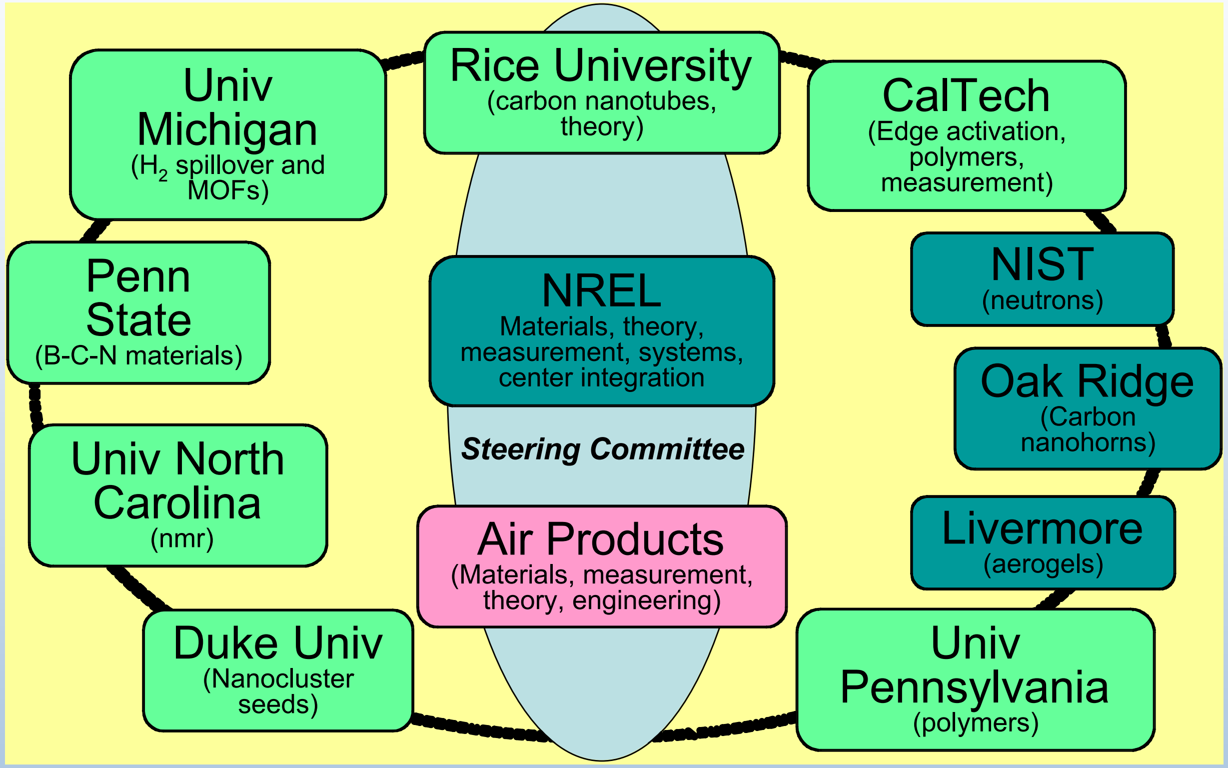
DOE Hydrogen Sorption Center of Excellence *(HS-CoE):* Overview

8 university projects (at 7 universities), 4 government labs, 1 industrial partner



DOE Annual Merit Review

May 15-18, 2007

This presentation does not contain any proprietary or confidential information

ST 1 and STP 5

Overview: Timeline and Budget

Timeline

- Center of Excellence start date: FY05
- Center of Excellence end date: FY09
- Percent complete: 40%

Budget

- Center funding
  - $27.5 M for five-year CoE
  - $2.5 M Contractor share (20% of Contractor budget)
- Management costs
  - ~243 K at NREL (~ 1 FTE)
  - ~33 K for Steering Committee

Barriers

- See next slide

Partners

Air Products (A. Cooper),
Duke (J. Liu),
CalTech (C. Ahn),
LLNL (J. Satcher),
NIST (D. Neumann,
NREL (M. Heben)
ORNL (D. Geohegan),
Penn State (P. Eklund),
Rice (J. Tour),
Rice (B. Yakobson, R. Hauge),
U. Michigan (R. Yang),
University of North Carolina (Y. Wu),
U. Penn. (A. MacDiarmid)
+ others outside of the COE

Prof. Alan G MacDiarmid
(1927-2007)

Overview: Barriers & Targets

General

- A. Cost.
- B. Weight and Volume.
- C. Efficiency.
- E. Refueling Time

Reversible Solid-State Material

- M. Hydrogen Capacity and Reversibility.
- N. Lack of Understanding of H Physi- and Chemisorption.
- O. Test Protocols and Evaluation Facilities.

Crosscutting Relevance

Compressed Gas Systems Barrier H: Sufficient Fuel Storage for Acceptable Vehicle Range.

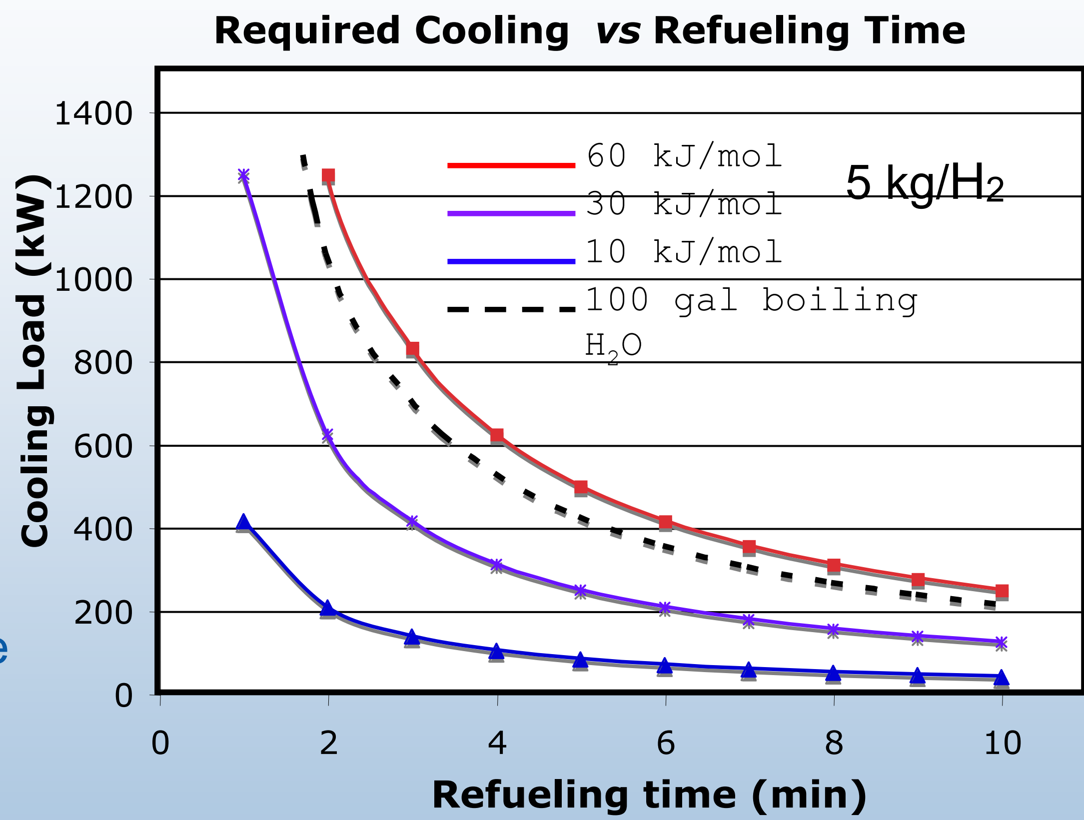
Off-Board Hydrogen Storage Barriers S & T: Cost and Efficiency

DOE 2010 Technical Targets for Storage System

- Gravimetric 0.06 kg H_2/ kg
- Volumetric 0.045 kg H_2/m^3

Approach: Binding Energy Impacts System Design

- High capacity is typically found with a high binding energy (E_B) and/or irreversible reactions.
- A large E_B makes charge & discharge inefficient, prohibits on-board refueling, reduces system capacities (heat exchangers), increases system and fuel/mile costs.
- An E_B which is too small reduces system capacities (insulation) & efficiency (compression & cooling), and increases system and fuel/mile costs.



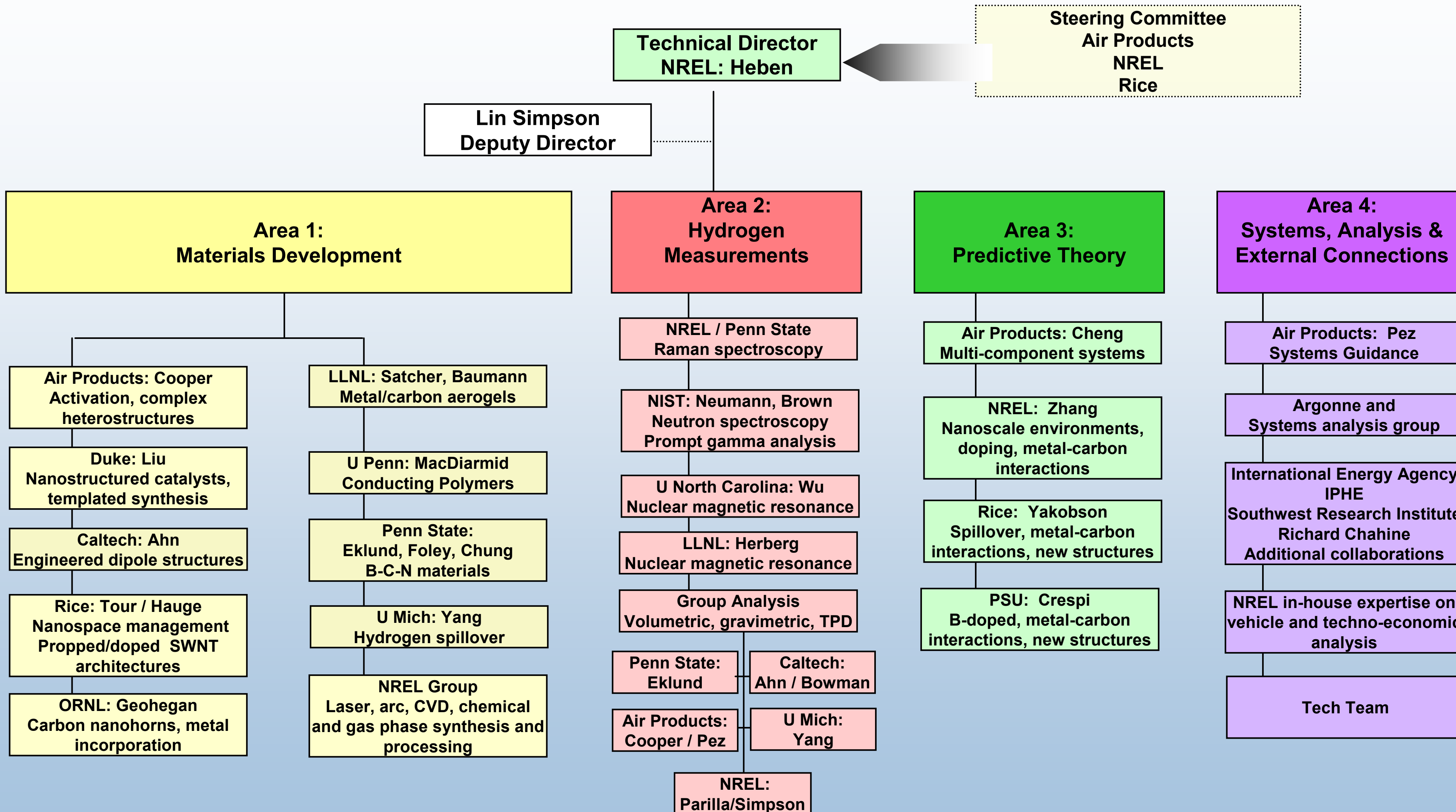
- **Optimized binding is essential to enable on-vehicle refueling and reduce overall costs**
- **Properly designed materials can have high capacities *and* desired intermediate binding energies (10 - 30 kJ/mol)**

Approach: Materials and Philosophy

- Develop hydrogen sorbents with high gravimetric/volumetric capacities and optimized E_B for on-vehicle storage.
- Design and synthesize materials which bind hydrogen as either (i) weakly and reversibly bound atoms or (ii) as strongly bound molecules.
- E.g. Boron/carbon polymers, MOFs, carbon nanohorns, aerogels, carbon-metal hybrid nanomaterials, new materials “built from the ground up”, non-carbon, new multi-component sorbents.
- Understand mechanisms and the interplay between structure, binding, and material stability and storage densities (per volume and per weight)
- Develop the experimental and computational tools to speed discovery, testing, and deployment of materials that meet DOE system goals.
- Create a collaborative, nimble environment to permit expeditious exploration, research, and deployment (sum of whole > sum of parts).
- Enable the development of new concepts and approaches.

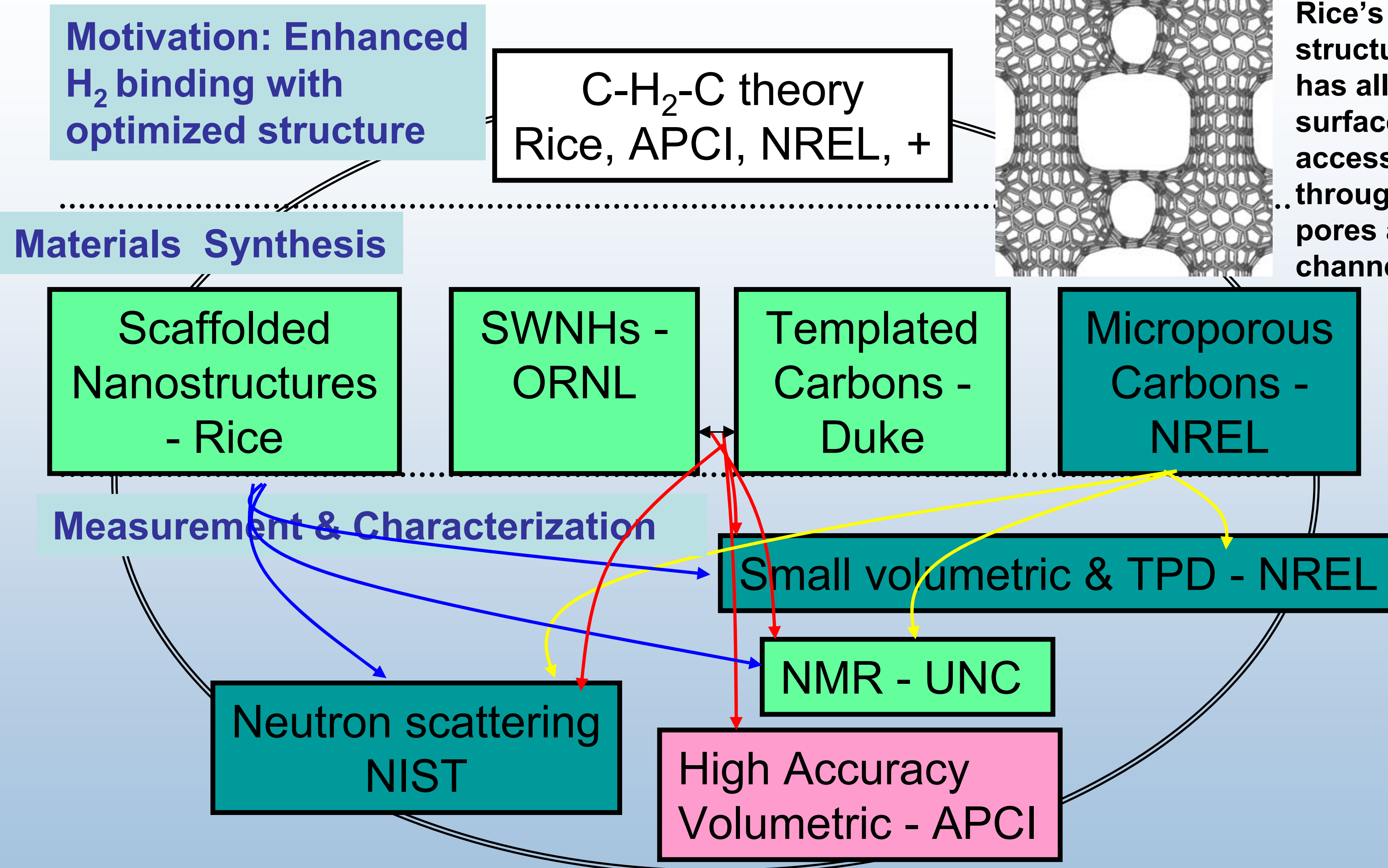
Effort is organized into disciplines and “clusters”. Clusters focus resources on synthetic efforts.

Approach: Center Organization



- Center is organized into five disciplines
- Collaboration across disciplines speeds development

CoE Accomplishment: Nanospace

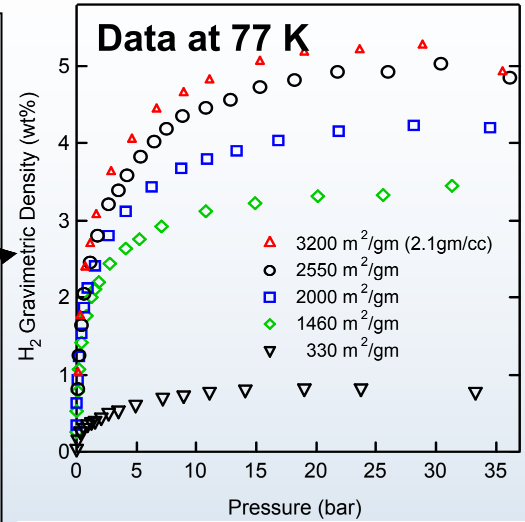


Rice's Nano-structured foam has all it's surface area accessible through open pores and channels.

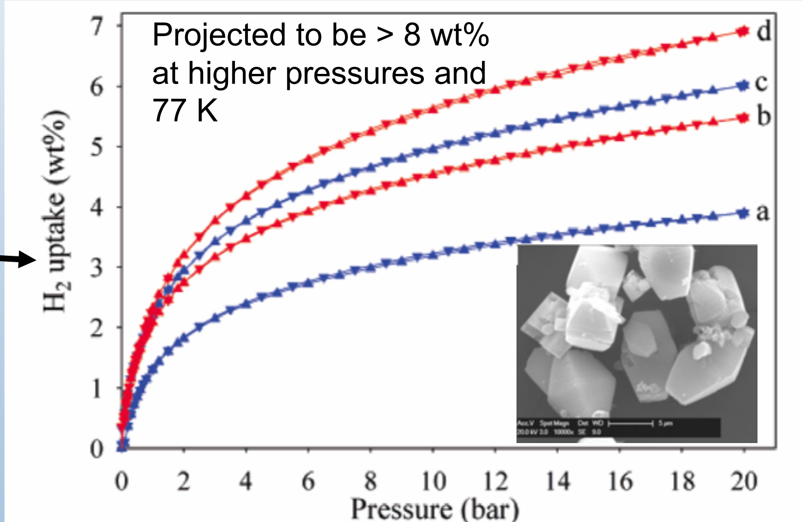
Research "Cluster" on designing Nanospace accelerates synthesis of high surface area materials with improved hydrogen storage capacities

Cluster Accomplishment: Enhanced Uptake per SSA

- High surface area is essential for high hydrogen storage capacities.
- Uptake per unit SSA is also important:
  - ACA: ~5 wt% per 2500 m^2/g
    - 1 wt% per 500 m^2/gm
    - 3200 m^2/gm for 2.1 g/cc material
  - MOF-177: ~7 wt% per 5900 m^2/g
    - >2x SSA, but only 40% increase in uptake, 1 wt% per 840 m^2/gm
- Optimal pore size could enhance uptake beyond that typically seen with SSA only:
  - e.g. Mokaya et al. Zeolite Templated Carbon, ~8 wt% per 3150 m^2/g
    - 1 wt% per 390 m^2/gm
    - Nano-engineered structure enhances uptake per SSA and total uptake beyond materials with higher SSA but larger pores
    - Will visit Mokaya (U. Nottingham) in June



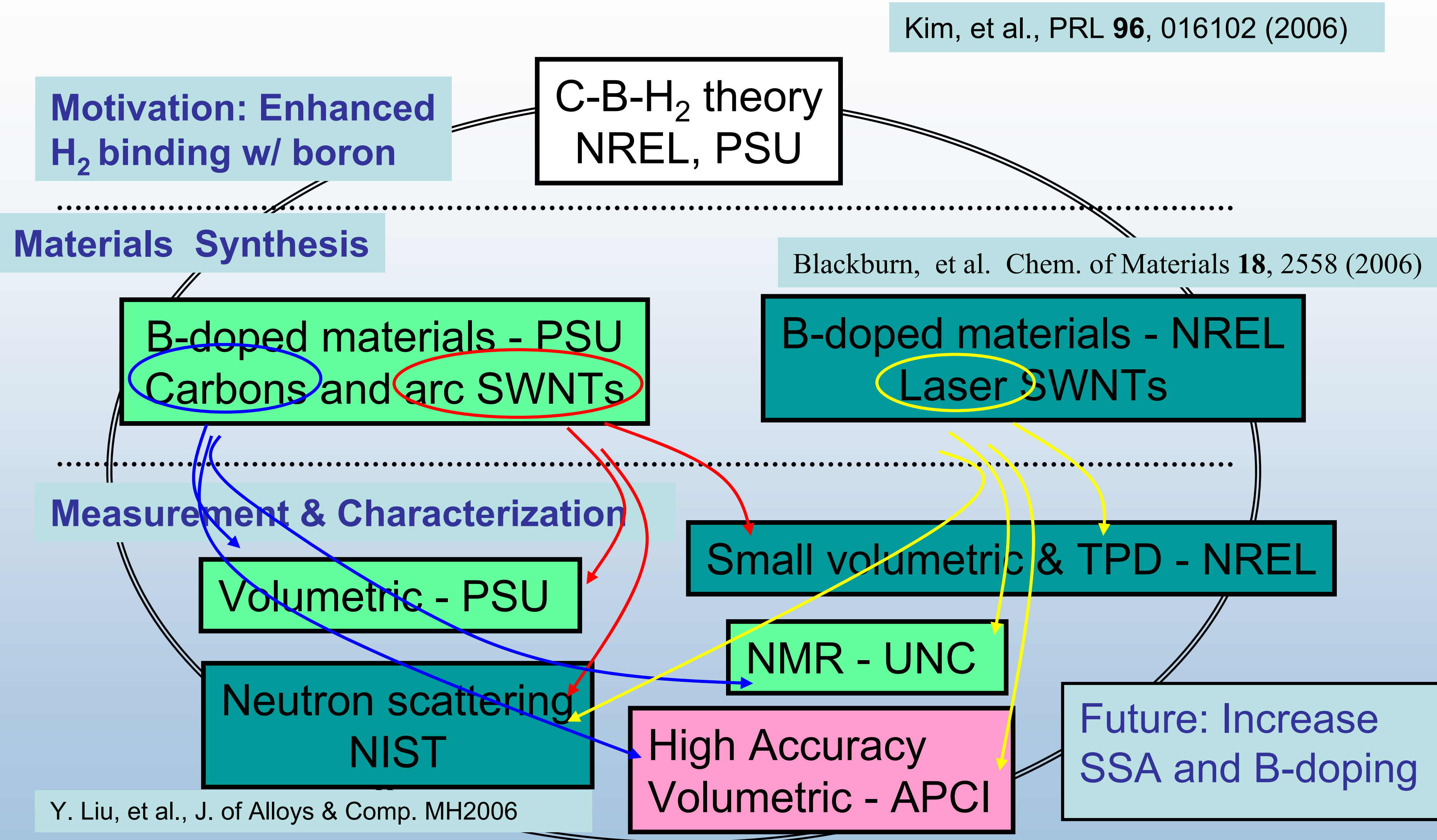
Activated Carbon Aerogel: Kabbour, Baumann, Satcher, Saulnier and Ahn, *Chem. Mater.* ***18***, 6085 (2006).



Zeolite Templated Carbon (~ 3150 m^2/g)
Z. Yang, Y. Xia, R. Mokaya *JACS* (2007)

Optimized structure enables higher uptake and SSA so that DOE 2010 system targets may be met at higher temperatures.

CoE Accomplishment: Dopants to Enhance Binding

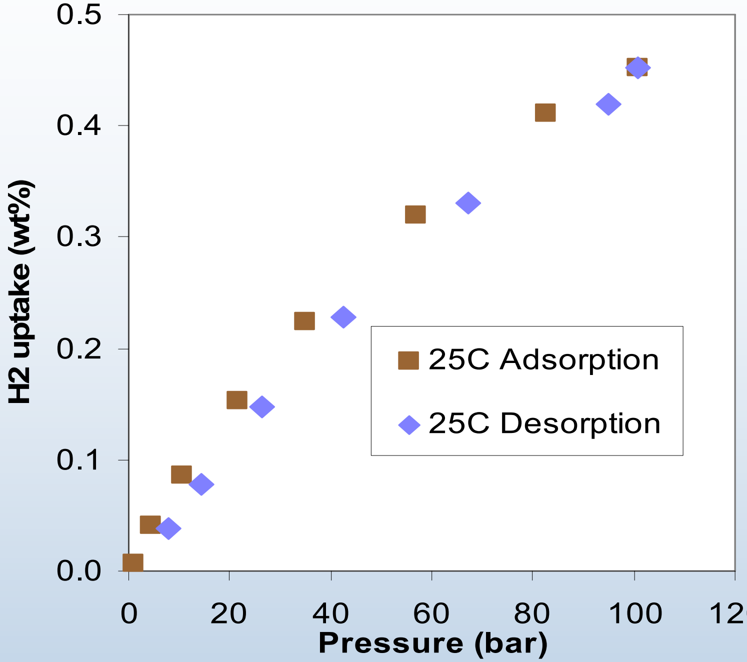


Cluster focused on Dopants accelerates efforts to synthesize materials with higher SSA and higher boron content (B doping increases E_B).

Cluster Accomplishment: Boron Doping

- Penn State increased B loading from 2 to 8 at% in sorbents derived from pyrolysis of polymers (Chung).
- 5 at% B material derived from molecular precursors (Foley) shows similar uptake at RT to activated carbon which has 2.5 times the SSA (950 m^2/gm *vs* 2500 m^2/gm).
- H_2 uptake at 77K for Chung material is ~50% higher than carbon with same SSA
- 9.2 kJ/mol H_2 (Wu), agrees with theory.
- Boron predicted by NREL and PSU to stabilize metal atom absorption to:
  - Improve spillover
  - Create solid-state Kubas complexes
- Next steps: Increase B loading with higher B content precursors, leverage CoE partners to enhance SSA .

Boron doped carbon (5 wt% B, 950 m^2/gm) from PSU (Foley)

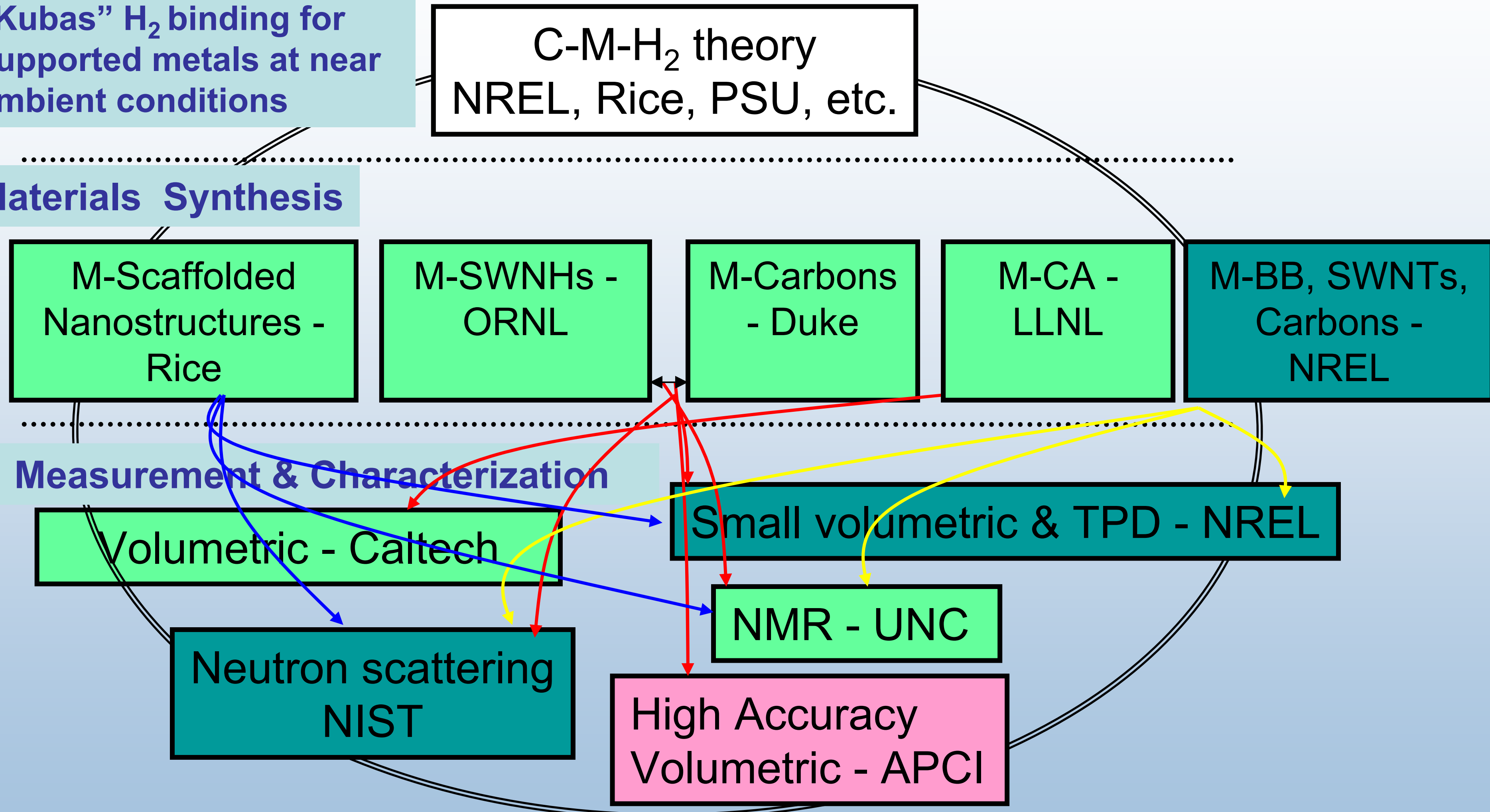


Boron enhances hydrogen binding when doped in carbon lattices and also stabilizes atomic metals to form Kubas sorbents - both promising routes to meet DOE targets under near ambient conditions.

CoE Accomplishment: Metal Binding

Motivation: Enhanced "Kubas" H_2 binding for supported metals at near ambient conditions

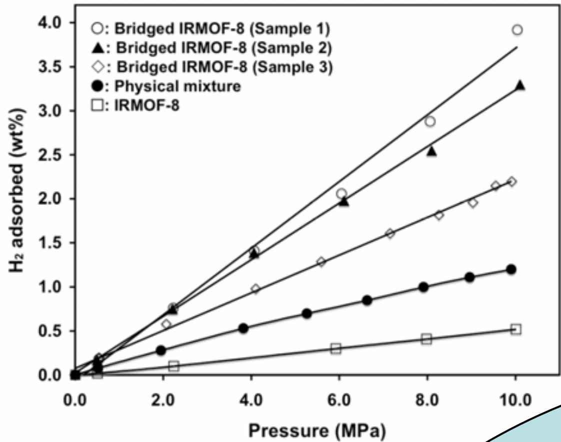
Y. Zhao CPL **425**, 273 (2006)



CoE leverages expertise to identify hydrogen storage approaches and focus synthetic efforts.

CoE Accomplishment: Spillover

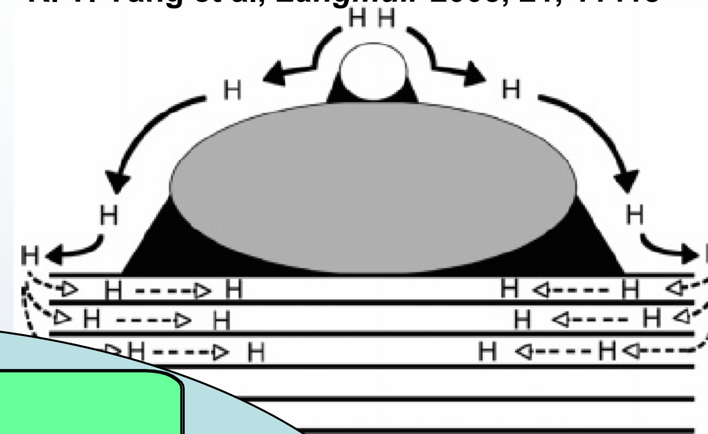
Isotherms measured at 298K on Pt/AC catalyst (10%) and IRMOF-8 (80 or 90%)



Li et al. JACS **128**, 8136 (2006)

UM developed phenomenological model of spillover. Diffusion on carbon matrix is the limiting factor, not dissociation.

Phenomenological spillover schematics
R. T. Yang et al, *Langmuir* 2005, 21, 11418



U Mich
Synthesis/measurement/theory

APCI
Theory

Rice
Theory

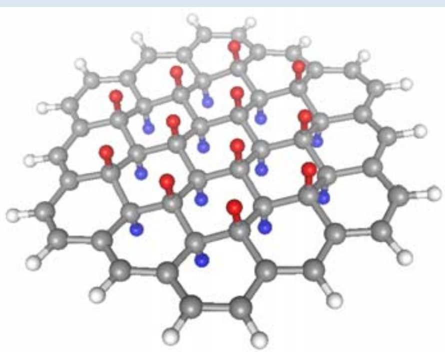
NREL
Volumetric/theory

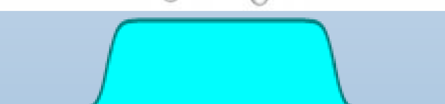
NIST
Measurement

UNC
Measurement

SWRI
Measurement

ORNL and Duke have also made materials that may show spillover

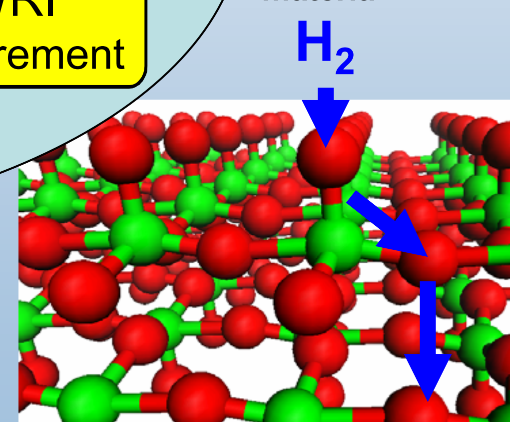




Rice calculations indicate that propagation front of H requires as little as 5 kJ/mol per H atom, compared to ~70 kJ/mol for an isolated H atom.

- Issues:
  - Stability of MOFs in spillover
  - Loss of spillover activation
    - Degassing processes observed to turn off spillover
    - Must develop better understanding

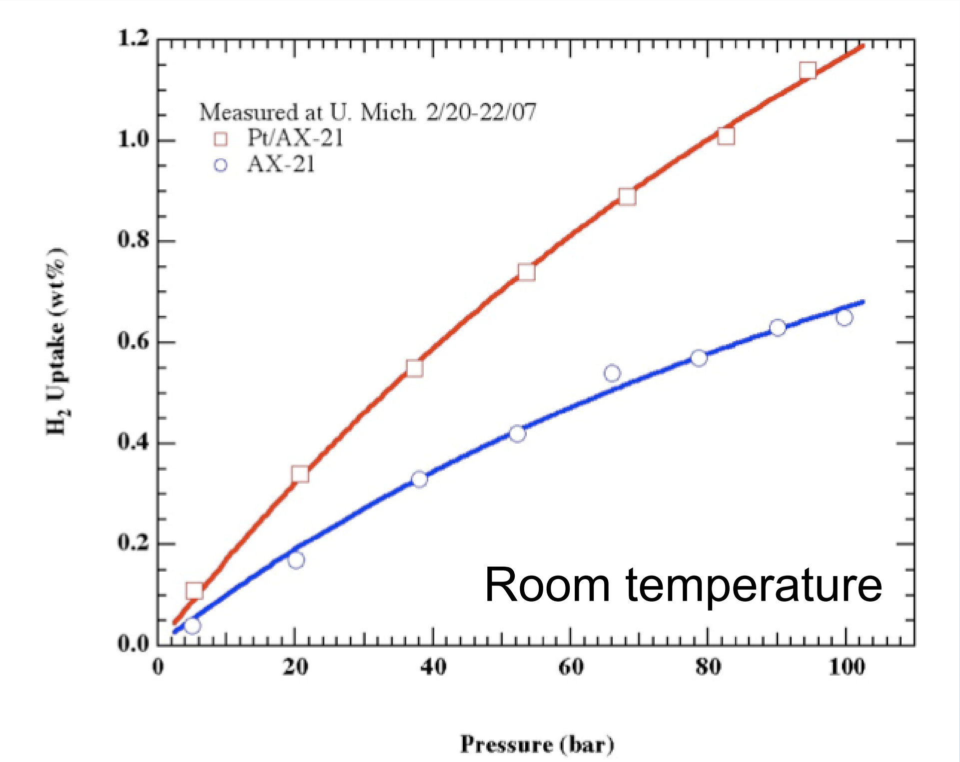
APCI models validated using "hydrogen bronze", a well known spillover material



$H_2 + MoO_3 \rightarrow H_xMoO_3$

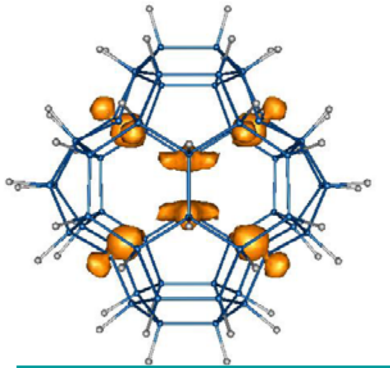
Spillover enables substantial RT hydrogen storage.

Cluster Accomplishment: Spillover
Validation of U. Michigan Result

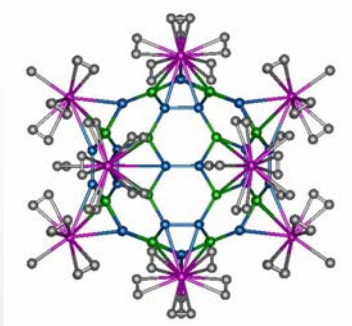


- **P. Parilla traveled to U. Michigan to observe simultaneous measurement (in two identical instruments) of AX-21 with and without Pt decoration**
- **Degas conditions and activation conditions are critical**
- **Replication of experiment at NREL is being pursued**

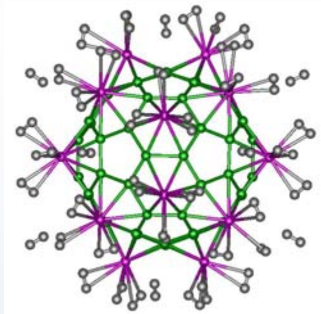
CoE Accomplishment: Materials Discovery



6.1 wt% $Ca_2@C_{60}H_{52}$

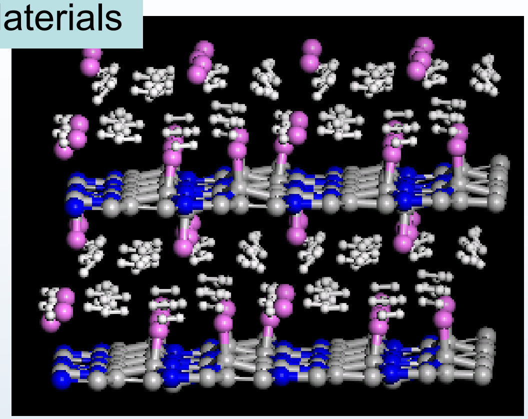


10.5 wt% $C_3B_2ScH_{12}$



8.6 wt % $B_{60}Sc_{20}H_{144}$

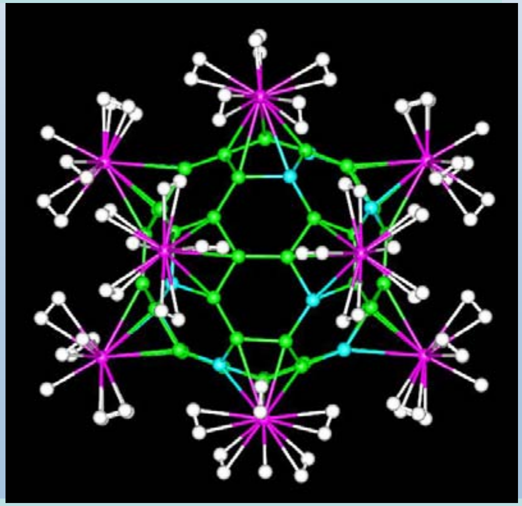
New Materials



~8 wt % $(C_6N_2)_n^{2n+}2nF^-$,
~20 kJ/mol H_2 ads. energy

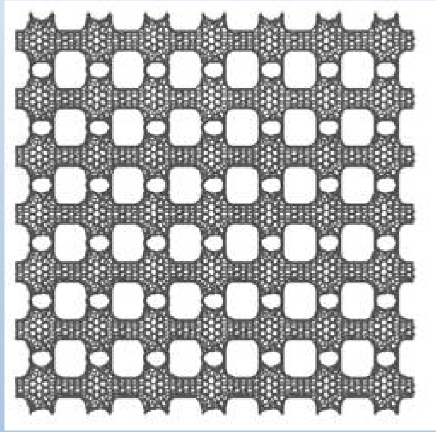
Endohedral Metallofullerenes
Y. Zhao et al. submitted (2007)
These materials are available.
(e.g. H. Dorn, VaTech)

NREL | APCI
PSU | Rice



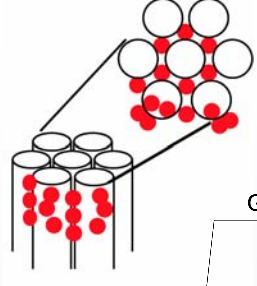
Synthesis of organometallic fullerenes is being pursued.
Y. Zhao et al. PRL **94**, 15504 (2005)

Theory and experiment iteratively interact:
- **Synthesis and measurement test theoretical approach**
- **Theory establishes targets for synthesis**

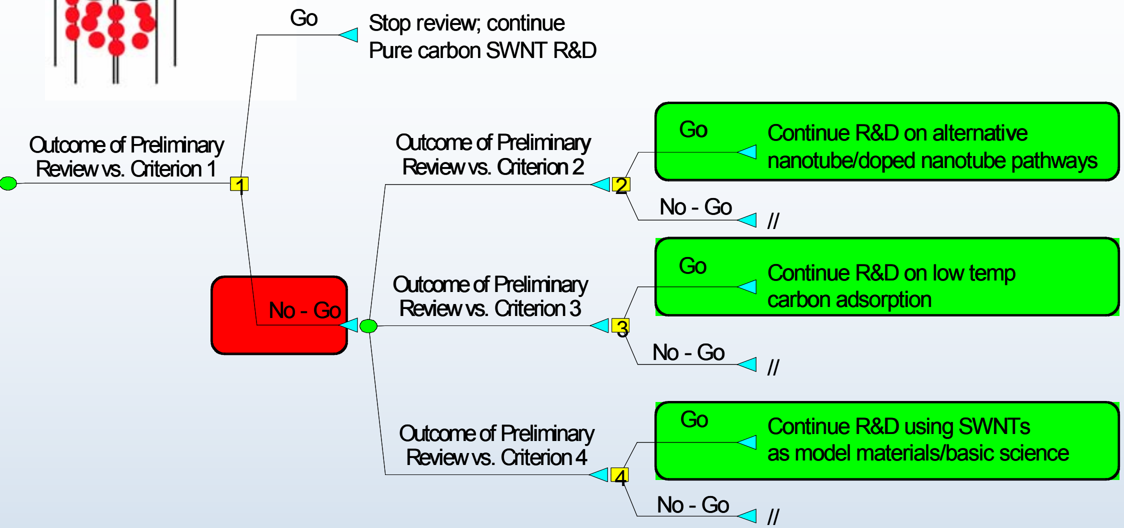


Rice's 3-D SWNT foam with nanometer diameter pores and channels (~2600 m²/g) is metallic and may have higher H2 binding due to structure

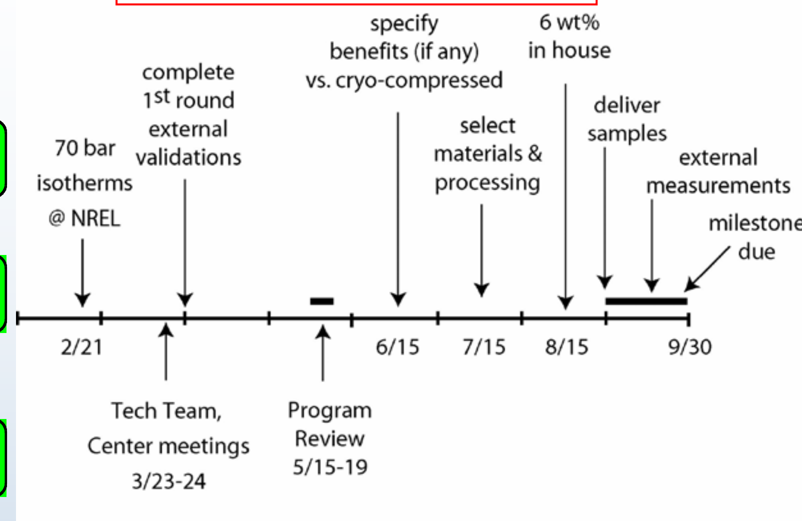
Down Select: SWNT No-Go Decision



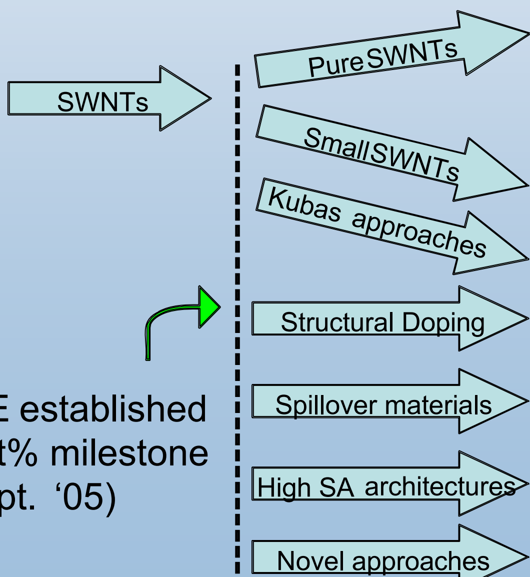
Decision Tree



Evaluation Process



Recommendation



Bulk, as producedSWNTs
- Recommend No Go

MOFs, aerogels, polymers, fullerenes, aerogels, zeolites, molecules, frameworks/supports, propped structures, doped structures, clathrates, metal-decorated and catalyzed carbons.
- Recommend Go for SWNT use as building blocks

CoE established 4 wt% milestone (Sept. '05)

Based on current evidence, pure SWNTs will not meet DOE 2010 storage system targets at ambient conditions. However, SWNTs may be an effective building block to construct viable sorbents

Down select: Partner GNG Recommendations

- HS CoE partners were evaluated for Phase 2
- Evaluations done in three parts:
  1. Discussion regarding milestone progress and programmatic goals with SC, GO, and HQ participation (Aug. 25th, 2006)
  2. SC members performed independent evaluation of each project with respect to:
     - Degree of collaboration and interaction
     - Technical progress with respect to stated goals
     - Preliminary Recommendation regarding transition from Phase I to Phase II
  3. Discussion of Evaluation and Recommendation with, and Solicitation of Feedback from, the Partner, DOE (HQ and GO), and the SC.
- Process took into account reviewer comments from Annual Program Review, and Tech Team input.
- Process is completed with a final recommendation for continuation or termination, and specific redirection requirements.

- **Preliminary recommendations for all partners have been completed.**
- **Working with each partner to complete recommendations, which may include suggestions for redirection to focus activities deemed important to DOE.**

Project Summary

Technical Accomplishments and Progress:

- Substantial interactions involving all partners were established to accelerate R&D.
- Strong teaming across institutions / topics / expertise.
- Optimized carbon pore structures enhances H_2 uptake, up to 8 wt% possible.
- Partner collaborations have enabled boron doped carbons that bind H_2 at ~ 12 kJ/mol: May enable ~RT and moderate pressure H_2 storage system.
- Boron doped carbons will more effectively hold metal atoms, limit aggregation.
- Metal-carbons synthesized and demonstrating unique sorption with higher binding.
- Partner collaboration have led to an improved understanding of spillover and development of additional materials.
- Demonstrated substantial (~5 wt%) irreversible hydrogen capacity of hybrids at STP.
- Materials discovery efforts have identified several new systems that could meet DOE targets and helped develop synthesis pathways to form others.
- Strong interplay between theory and experiment is identifying weaknesses in approaches, and determining new paths forward.
- Organization and management of Center has actively guided efforts.
- Regular technical exchange meetings on focused topical areas.
- Steering Committee has provided direction and developed partner Phase 2 go/no-go recommendations.
- At least 72 publications, 87 presentations, and 2 patents

For other Progress, see talks and posters from CoE partners!

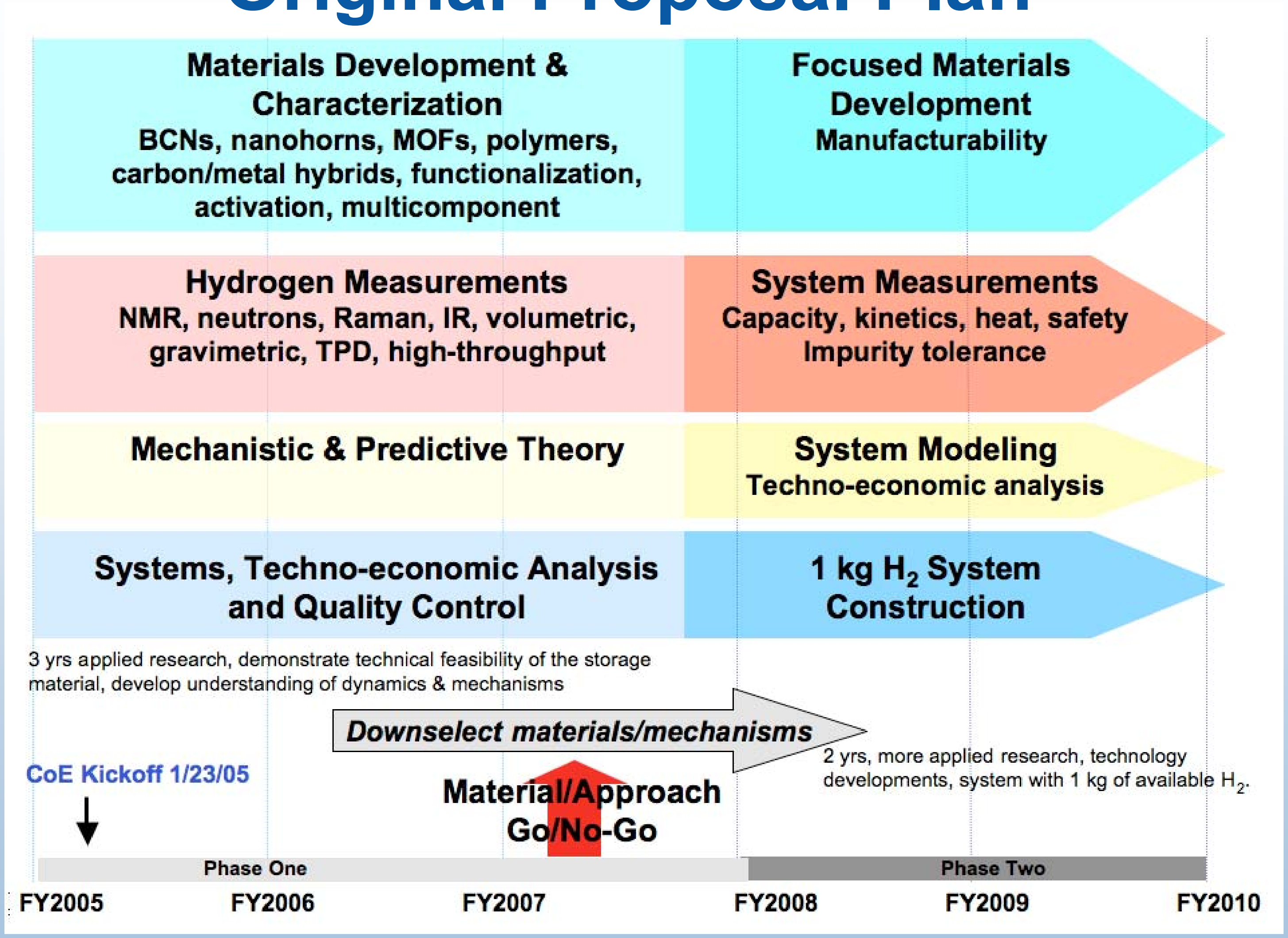
Future FY07 Work

- Complete customization of commercial high pressure volumetric system for use in laboratory scale (~10 mg samples) analysis to help accelerate materials development. Transition to community.
- Complete validation of spillover results (controlled activation).
- Transition, redirect, or terminate polymer project.
- Continue developing processes to nano-engineer hybrid materials
  - Demonstrate TM-C_{60} materials that have appropriate structures similar to theoretical predictions. Complete link between theory and experiment.
  - Identify/demonstrate synthesis of other new materials.
    - Demonstrate TM-SWNT, Catalyst-SWNT, and Alkali metal-carbon structures with room temperature hydrogen sorption significantly higher than the base materials.
    - e.g. Pt/Pd decorated carbons with 2-4 X increase in hydrogen sorption at ~ RT.
  - Integrate work with other spillover and materials development activities in the COE.
- Perform calculations to identify new materials that could meet DOE targets
  - Complete calculations investigating the affects of alkali metal with carbon to bind H_2
  - Complete initial models for spillover in the MetCar systems. Apply to other cases.
  - Accelerate analysis of multi-component and non-carbon systems.
- Continue Center activities to accelerate H_2 storage materials development
  - Work with others to provide rapid materials characterization and develop new materials
  - Work with DOE/GO to ensure optimum functioning of the Center
- Stop unproductive directions and integrate new CoE Projects.

FY08 Work

- Develop new lab scale testing to accelerate H_2 materials development
  - e.g. H_2 BET surface area measurements that accurately correlate to H_2 capacity
- High pressure and high temperature optical spectroscopies to elucidate stability, activation, and mechanistic issues.
- Develop materials with intrinsically high surface areas
  - e.g. CVD replica generation of zeolitic templates
  - e.g. New MOF materials
  - e.g. Nano-engineered carbon structures with enhanced binding (> 10 kJ/mol)
  - Propped structures, foams
- Improve reversibility of hybrid materials
- Develop synthetic methods to increase Boron concentrations
- Advance synthesis of more tractable TM-carbon Kubas materials and multi-component and non-carbon sorbents
- Improve fundamental understanding of different sorption processes
- Search for sorbent materials, both experimentally and computationally, which can be readily synthesized and will likely be stable.
- Coordinate Center activities to accelerate H_2 storage materials development
  - Work with others to provide rapid materials characterization and develop new materials / approaches.
  - Work with DOE/GO and partners to ensure optimum functioning of the Center
  - Redirect activities away from unproductive materials and approaches toward more productive ones.
- Adjust Center timeline

Original Proposal Plan



- CoE is on-time with respect to original plan.
- Magnitude of challenge precludes moving to 1 kg system design next year.
- Applied research will continue while keeping apprised of advances in relevant system designs (e.g. metal hydride systems).

Summary Table of Selected HS COE Results

Materials Performance																			
Storage Parameters	Units	System Targets (2010)	MOF-177[a] (UM/ UCLA)		Spillover (UM)		SWNTs (NREL)		M-C_{60} (NREL)		Aerogels (LLNL)			Pt-SWNH (ORNL)		Reduced Carbons[d] (NREL)		B-doped Carbons[e] (PSU)	
			FY05	FY06	FY05	FY06	FY05	FY06	FY06	FY07	FY06	FY07	FY07	FY06	FY07	FY06	FY07	FY06	FY07
Specific Energy	Wt% H2	6	2.5	7	1.6	~4	b	3	0.5	0.5	4.2	5.3	>8[c]	1	2.5	4.2	5	*	3.2
Volumetric Energy Capacity	g/L	45	*	31	*	41	*	28	*	*	*	29	*	*	*	*	*	*	*
Comments			77 K, 50 bar	77 K, 60 bar	RT, 100 bar	RT, 100 bar		77 K 20 bar	77K 2 bar	STP	77 K, 30 bar	77 K, 30 bar	STP	77K 10 bar	77 K 10 Bar	STP	STP		77 K, 30 bar

* Information not available
Volumetric capacities derived from material densities
a. Wong-Foy et al., JACS 128, 3494 (2006)
b. Prior to 2006, SWNT hydrogen uptake results have not been reproduced at different labs. 4 to 6 wt% results reported.
c. When loaded with LiBH4, the aerogel as a scaffold lowered the desorption temperature to ~ 400C.
d. Materials developed at NREL are mostly irreversible since a dissociation component has not yet been incorporated.
e. Boron binding sites demonstrated ~ 10 KJ/mol, close to theoretical predictions. SSA needs to be increased (~800 m2/g)
f. Note that outside the center, ~ 5 wt % (77K and 90 bar) and ~8 wt% (77 K and ~100 bar) were demonstrated with MOFs by M. Dinca et al. JACS 128, 16876 (2006) and templated carbons by Z. Yang et. al. JACS 1021/ja067149g (2007), respectively.

Summary Table: Predicted HS Results

Theoretical Materials Predictions									
Storage Parameters	Units	System Targets (2010)	Organo-metallic Fullerenes [a] (NREL)	MetCars [b] (NREL)	Macro-molecules (NREL)	Endohedral Metallo-fullerene[c]	Metallo-carborane[d] (NREL)	$(C_6N_2)_n^{2n+}$ $2nF^-$ (APCI)	Spillover on SWNT (NREL)
			FY05	FY06	FY06	FY07	FY07	FY07	FY06
Specific Energy	Wt% H2	6	~9	3.7-7.7	>5	6.1	10.5	7.4[e]	>7.7
Volumetric Energy Capacity	g/L	45	52-43	48-58	>40	*	52	*	~56
Comments			STP, 23-46 kJ/mol	STP, 15-32 kJ/mol	STP	~STP, 10-78 kJ/mol	STP	~STP, ~20 kJ/mol	RT, 100 bar

* Information not available

Volumetric capacities derived from material densities

a. Zhao etal. PRL 94, 15504 (2005). Similar predictions have appeared in the literature including, Yildirim and Ciraci, PRL 94, 175501 (2005); Shin, Yang, Goddard III, and Kang, APL 88, 053111 (2006); Deng et al. PRL 92, 166103 (2004); Lee, Choi, and Ihm, PRL 97, 056104 (2006); Q. Sun et al., J. Am. Chem. Soc. 128, 9741 (2006).

b. Chem. Phys. Lett. 425, 273 (2006).

c. Y. Zhao et al. submitted to JACS, NREL.

d. Initial calculations performed at NREL.

e. Initial calculation performed by APCI.

Internal HS CoE Collaborations

1. “Sorption behavior in high surface area carbon aerogels." Primary contacts: Channing Ahn (Caltech) and Ted Baumann (LLNL), Oct 2005 to May 2007.
2. ”Sorption behavior in carbon nanohorns." Primary contacts: Channing Ahn (Caltech) and David Geohegan/ Hui Hu (ORNL), Mar 2006 to May 2007. Hydrogen isotherm study showed ~2.5 wt% hydrogen uptake of opened SWNHs at 77K, which is three times of that of unopened AP-SWNHs.
3. “Neutron diffraction in a high sorption enthalpy MOF-74 compound" Primary contacts: Channing Ahn (Caltech), Craig Brown (NIST), Mar 2007 to May 2007.
4. “Hydrogen sorption measurements at NREL on LLNL carbon aerogel material.s” Primary Contacts: T. Baumann (LLNL) and P. Parilla (NREL). November 2006. Room temperature hydrogen adsorption measurements performed on CA materials.
5. “Characterization of LLNL carbon aerogels at NIST using neutron scattering techniques.” Primary Contacts: T. Baumann (LLNL) and C. Brown (NIST). March 2007 to present. Characterization of carbon aerogel materials using small angle neutron scattering and hydrogen spectroscopy.
6. “Spillover catalyst studies at CalTech on LLNL metal-loaded carbon aerogel materials.” Primary Contacts: T. Baumann (LLNL) and C. Ahn (CalTech). November 2006 to present. Reduction of metal ions (Ni and Pt) impregnated in high-surface-area carbon aerogels, characterization of aerogel-supported catalyst nanoparticles and hydrogen uptake measurements on metal-loaded carbon aerogels.
7. “NREL BET, Volumetric and TPD Measurements of Duke small diameter carbon nanotubes and other materials.” Primary contacts: Jie Liu (Duke) and Lin Simpson (NREL), Feb 2006 to January 2007. Hydrogen uptake measurements provided information for effect of nanotube diameters on storage capacity.
8. “Growth of nanotubes with controlled diameters” Primary contacts Jie Liu(Duke) and Bob Hauge (Rice), Feb. 2006 to Jan. 2007. Discussion on the effect of growth conditions on the diameter of carbon nanotubes. Discussion on the growth mechanism of carbon nanotubes.
9. "Measurement of the binding energy of hydrogen on microporous carbon materials using NMR", Primary contacts Jie Liu(Duke) and Yue Wu(UNC), Dec. 2006 to now. Discussion and planning on measuring the binding energy of hydrogen on microporous carbon materials to understand the potential for hydrogen storage.
10. "Study the binding of hydrogen on carbon nanotubes materials using neutron ", Primary contacts Jie Liu(Duke) and Yun Liu (NIST), May 2006 to Jan 2007. Provided samples to NIST for testing the binding of hydrogen on nanotubes with metal decoration.
11. “NREL Hydrogen Sorption Capacity Characterization, TPD and C NMR Measurements of ORNL Single Walled Carbon Nanohorn (SWNH) Materials." Primary contacts: Hui Hu (ORNL) and Lin Simpson (NREL), Anne Dillon (NREL), Jeffrey Blackburn (NREL), and Chaiwat Engtrakul (NREL), December 2005 to April 2007. Initial tests of the opened Pt-SWNHs indicated ~ 1.4 wt% hydrogen sorption with an over pressure of 2 bar at liquid nitrogen temperatures. TPD data on opened Pt decorated SWNHs has shown a hydrogen peak at around room temperature, with a binding energy of ~36 kJ/mol.
12. “NIST Neutron Scattering, PGAA, and Hydrogen Isotherm Measurement of ORNL SWNH Materials.” Primary contacts: Hui Hu (ORNL) and Yun Liu (NIST). December 2005 to March 2007. Neutron scattering data provided the proof of “spillover” effect of metal (Pt, Pd) decorated SWNHs.
13. “University of North Carolina 1H NMR study of ORNL SWNH Materials.” Primary contacts: Hui Hu (ORNL) and Alfred Kleinhammes (UNC). December 2005 to April 2007. 1H NMR of Pt-SWNHs indicated the presence of adsorption sites with 0.8 wt% at RT. The nature of this binding site is still under investigation. Also measured adsorption at 80 K and found a Langmuir type of adsorption at a level of 1.5 wt%. The corresponding binding energy is 7 kJ/mol.
14. “Air Products and Chemicals, Inc. Hydrogen Isotherm Measurement of ORNL SWNH Materials.” Primary contacts: Hui Hu (ORNL) and John Zielinski (Air Products). December 2005 to March 2006. Hydrogen uptake measurement of SWNHs.
15. "Hydrogen adsorption study of B-substituted C (B/C) materials at NREL. Primary Contacts: Mike Chung (Penn State) and Jeffery Blackburn, Lin Simpson, Michael Heben (NREL), February to June 2006. Hydrogen adsorption of B/C material (5.7% B content; 528 m2/g SSA) at low hydrogen pressure (2 bar) shows ~ 1.5 wt% hydrogen uptake, significantly higher than that of the corresponding C.
16. "Elemental analysis of B/C materials by Prompt Gamma-ray Activation Analysis (PGAA)" Primary Contacts: Mike Chung (Penn State) and Yun Liu, Craig Brown, and Dan Neumann (NIST), February to September 2006. The PGAA measurement provides the precise B content. This collaboration is very important in developing suitable B/C precursors and pyrolysis conditions.
17. "Solid state 11B NMR and in situ 1H NMR studies of hydrogen adsorption on B/C samples" Primary Contacts: Mike Chung (Penn State) and Alfred Kleinhammes, Yue Wu (UNC), February 2006 to April 2007. This study provided direct evidence for hydrogen adsorption on B/C materials and the enhanced binding energy (~ 10 kj/mol).

Internal HS CoE Collaborations (continued)

18. "Air Products (AP) High Pressure Hydrogen Adsorption Measurements of Penn State University (PSU) Boron-containing Graphitic Carbons". Primary contacts: John Zielinski (AP) and Mike Chung (PSU), Summer 2006-Fall 2006. Hydrogen uptake measurements on 2 samples provided information on effect of boron levels and surface area on hydrogen adsorption properties.
19. "Hydrogen sorption capacity characterization at NREL of PENN STATE Boron doped NPC samples" Primary Contacts: Henry C. Foley (Penn State) and Lin Simpson (NREL) November 2006 to March 2007. Hydrogen sorption results showed that B-doped samples had much higher hydrogen uptake than activated carbon with similar surface area.
20. "Room temperature Hydrogen sorption studies at APCI of PSU Boron doped NPC samples." Primary Contacts: Henry C. Foley (Penn State) and John Zielinski (APCI) August 2006 to April 2007. Hydrogen uptake measurements at room temperature showed enhancement in uptake due to the presence of boron in NPC.
21. "NMR studies of PENN STATE Boron doped NPC samples" Primary Contacts: Henry C. Foley (Penn State) and Alfred Kleinhammes (UNC) February to March 2007. NMR measurements are going to provide information on binding sites and binding energies.
22. "Investigation of collective stabilization effects and enthalpic crossover for H adsorbed to graphene surfaces as a function of coverage." primary Contacts: Boris Yakobson (Rice) and Vincent Crespi (PSU), 2006-2007.
23. "Kubas' metal clusters," Primary Contacts: B. Yakobson (Rice) and Y. Zhao (NREL), 2005-present. Investigate metal clusters on tubes and extended graphitic support with emphasis on stability w.r.t. aggregation of metal.
24. "Locating Hydrogen binding sites in MOF-74." Primary contacts: Dan Neumann (NIST) and Boris Yakobson (Rice), Nov. 2006 to Jan 2007. Estimates of vibrational frequencies given.
25. "Atomistic simulations and understanding of spillover at Rice University." Primary contacts: Boris Yakobson (Rice) and Ralph Yang (University of Michigan), August 2006 to present. Yakobson's simulations help understanding of the experimental results on spillover done at Michigan.
26. "Comparison of curvature-effect," Primary Contacts: B. Yakobson (Rice) and H. Cheng (APCI), 2006-present.
27. "Collaboration on carbon scaffold development." Primary contacts: Boris Yakobson (Rice) and J. Tour (Rice), 2006-2007.
28. "Searching for enhanced hydrogen interactions in boron substituted carbons." Primary contacts: Craig Brown (NIST) and Jeff Blackburn (NREL), Jan 2006 to Jan 2007. Boron content was deemed to be too low to determine an enhanced interaction.
29. "TPD characterization of spillover sorbents at NREL." Primary contacts: Mike Heben and Phil Parilla (NREL), and Ralph Yang (University of Michigan), August 2006 to May 2007. New desorption peaks observed in the wide temperature range of 100-300K. The data at Michigan on spillover (Pt/AX-21) were validated.
30. "Searching for spillover on metal doped activated carbon." Primary contacts: Craig Brown (NIST) and Ralph Yang (Michigan), Apr 2007 to now. The hydrogen stored on a stable spillover sorbent (prepared at Michigan) is being characterized by neutron scattering at NIST.
31. "Search for enhanced hydrogen interactions in boron doped-SWNTs." Primary contacts: Jeff Blackburn (NREL) and Y. Wu (UNC), Jan. 2006 to present.
32. "Validation of hydrogen storage capacity with NMR." Primary contacts: Y. Wu (UNC) and A. Cooper (APCI), 2006-present.
33. "BET, Volumetric and TPD Measurements of PENN Conducting Polymer Materials." Primary contacts: Alan MacDiarmid (PENN) and Erin Whitney (NREL), May 2006 to January 2007. Measurements provided information for refining the conducting polymer processing and determine their H2 storage properties.
34. "NMR studies of Polyaniline Nanofibers." A. MacDiarmid (Penn) and Y. Wu (UNC), 2006.
35. "Room temperature Hydrogen sorption studies at APCI of NREL Boron doped SWNT samples." Primary Contacts: Jeff Blackburn (NREL) and John Zielinski (APCI) August 2006 to April 2007.
36. "NREL BET, Volumetric and TPD Measurements of Rice SWNT Scaffold Materials." Primary contacts: James Tour (Rice) and Lin Simpson (NREL), May 2006 to May 2007. Rapid feedback of the hydrogen uptake properties of small SWNT laboratory samples enables accelerated process development to prop open SWNT bundles and build scaffolded structures where hydrogen can access all the carbon surface area in a configuration that potentially has higher binding energies.

External HS CoE Collaborations

1. “Hydrogen sorption properties of MIL-53, 100 and 101 compounds" Primary contacts: Channing Ahn (Caltech) and Anne Dailly (GMR&D), June 2006 to May 2007.
2. “Development of aerogel materials as scaffolds for metal hydride systems” Primary Contacts: T. Baumann (LLNL) and J. Vajo (HRL, MHCoE). June 2006 to present. Design of aerogel scaffolds (both carbon and metal oxide) to improve the performance of metal hydrides systems, such as $LiBH_4$ or MgH_2.
3. “Carbon aerogels as scaffolds for sodium alanate” Primary Contacts: T. Baumann (LLNL) and R. Bowman (JPL, MHCoE). March 2007 to present. Investigation of cycling performance of $NaAlH_4$ supported in carbon aerogel scaffolds.
4. “Atomic layer deposition of metals on aerogel substrates” Primary Contacts: T. Baumann (LLNL) and S. Bent (Stanford). September 2006 to present. Development of atomic layer deposition techniques for the controlled deposition of catalytic metal nanoparticles on the inner surfaces of carbon aerogel substrates.
5. “ORNL BET, Hydrogen Isotherm Study of ORNL SWNH Materials.” Primary contacts: Hui Hu (ORNL), Nidia Gallego (ORNL) and Cristian Contescu. 4/06 to 5/07.
6. “Grand Can Monte Carlo capacity computations,” B. Yakobson (Rice) and Rachel Aga (ORNL), 2006-present.
7. “NMR study of modified MOF.” Primary contacts: Yue Wu (UNC-Chapel Hill), Samuel Mao (Berkeley and LBNL) Performed room temperature measurement of modified MOF from LBNL.
8. “Understanding structure and dynamics, and locating H2 binding sites in MIL-53.” Primary contacts: Craig Brown (NIST) and Anne Dailly (GM), Jan 2007 to now.
9. “Locating Hydrogen binding sites in MOFs of tunable pore size.” Primary contacts: Craig Brown (NIST) and Gavin Walker (Uni. Nottingham U.K.), Feb 2007 to now.
10. “Locating Hydrogen binding sites in PCN materials.” Primary contacts: Yun Liu (NIST) and Shengqian Ma (Uni. Miami, Ohio), Nov 2006 to now.
11. “Searching for Hydrogen spillover in activated carbons.” Primary contacts: Craig Brown (NIST) and Christian Contescu (ORNL), Nov 2006 to now.
12. “Enhanced hydrogen binding in unsaturated metal centered MOFs.” Primary contacts: Craig Brown (NIST) and Jeff Long (UC Berkeley), Jan 2006 to now.
13. “Understanding hydrogen binding in HKUST-1.” Primary contacts: Craig Brown (NIST) and Vanessa Peterson (ANSTO, Australia), Jan 2006 to now.
14. “Gravimetric Measurements of Conducting Polymer Materials.” Primary contacts: A. MacDiarmid/P-C Wang (PENN) and A. Ignatiev (U Houston), 2006 to Feb. 2007.
15. “ SEM of PENN Conducting Polymer Materials.” Primary contacts: Alan MacDiarmid/P-C Wang (PENN) and A. Wu (UT-Dallas), February 2007 to March 2007.
16. "LRSM, Thermoanalysis of Conducting Polymer Materials.” Primary contacts: A. MacDiarmid/P-C Wang (PENN) and A. McGhie (PENN LRSM), Fall 2006.
17. “H2 interactions with Cond. Polymers Using Electronic Nose Devices.” Primary contacts: A. MacDiarmid/P-C Wang (PENN) and A.T. Johnson (PENN), summer 2006.
18. "Air Products (AP) High Pressure Hydrogen Adsorption Measurements of Miami University of Ohio (MU) Metal-organic Framework Materials". Primary contacts: John Zielinski (AP) and Hong-Cai (Joe) Zhou (MU), Summer 2006-Spring 2007. Hydrogen uptake measurements samples provided information on metal unsaturation and surface area effects on hydrogen adsorption properties.
19. "Air Products (AP) High Pressure Hydrogen Adsorption Measurements of Penn State University (PSU) Ga/Ge Sodalite and LiCHA zeolite materials.". Primary contacts: John Zielinski (AP) and David Vaughan (PSU), Fall 2006. Hydrogen uptake measurements provided information on effect of cation exchange in zeolites on hydrogen adsorption properties.
20. "Volumetric and Raman Measurements of Nanoporous Carbons.” Phil Parilla and Anne Dillon (NREL) and Peter Pfeifer (University of Missouri) June, 2006 - Oct. 2006. Measured the H2 capacities and Raman spectra of nanoporous corncob derived carbon samples. The measurements validated the viability for hydrogen storage.
21. “ BET specific surface area (SSA) and single point hydrogen sorption measurements of Mn acetate tetrahydrate (MnOR) samples.”Primary Contact Mike Heben and Lin Simpson (NREL), and Doug Schulz (North Dakota State University).
22. “Hydrogen sorption measurements of SiOC and SiBOC samples.” Primary contacts: Mike Heben and Lin Simpson (NREL), and Dr. Alonso (U. Trento (Italy)), Fall 2006.
23. “Hydrogen uptake measurements of PANI from Aerospace Corp.” Primary Contacts: Mike Heben (NREL) and Bruce Weiller (Aerospace Corp.) Fall 2006
24. “Hydrogen adsorption on nanocrystalline metals and alloys.” Jeff Blackburn and Kevin O’Neill (NREL), and Garry Glaspell (Virginia Commonwealth University), Fall 2006 to Spring 2007. Performed TPD and volumetric adsorption on a variety of nanocrystalline metals and alloys to ascertain if size effects lead to improved kinetics, desorption temperatures, or capacities of the metals and alloys.
25. “Hydrogen adsorption on titanium-filled single-wall carbon nanotubes.” Jeff Blackburn (NREL) and Leonid Grigorian (YTCA America in Camarillo, CA), Fall 2006. Performed TPD measurements on several samples; i.e. (SWNTs) filled with several titanium solid phases.
26. U. Houston: Worked with NREL and U.Penn to valid storage measurements on conducting polymers. Alex Ignatiev with U.Penn and NREL Staff
27. Virginia Tech and NREL: Endohedral Fullerenes for hydrogen storage. Calculations and joint BES proposal. Primary Contacts: Harry Dorn, Mike Heben
28. University of British Columbia and Hydrogen Storage Media, Inc.. NREL performed desorption measurements on AlH4 & NaAlH4 (Keyser, McGrady, Willson, Heben)
29. University of Colorado. NREL assisted Rishi Raj in developing a CU program on H2 storage using polymer derived ceramics (Raj, Heben).

NREL Services

1. Anne Dillon is leading the organization of a session entitled "The Hydrogen Economy" at the spring 2008 MRS meeting in San Francisco.
2. Anne Dillon is co-organizing a Symposium entitled "Life-Cycle Analysis" at the Materials Research Society (MRS) Fall Meeting, Boston, MA Nov. 26-30, 2007.
3. Anne Dillon is on the International Organizing Committee for the "International Symposium on Materials Issues in a Hydrogen Economy" to be held in Richmond, Virginia during November 12-15, 2007.
4. M.J. Heben co-organized a session on “Hydrogen Production, Transport, and Storage 2” at the ECS meeting in Chicago (May 6 -11, 2007).
5. M.J. Heben co-organized a symposium at the MRS Fall meeting, Boston, MA, in November 2006
6. M.J. Heben submitted a research plan for NREL's participation in a joint project with Richard Chahine (University of Quebec, Trois Rivieres) for the new IEA Annex 22
7. Anne Dillon interacted with and served on the International Program Committee for the 4th International Conference on Hot-Wire CVD (Cat-CVD) Process, Takayama, Japan, October 4-8, 2006.
8. Anne Dillon participated in The National Academy of Engineering's U.S. of Frontiers of Engineering Symposium, Dearborn, MI, Sept. 21-23, 2006, discussing energy related topics.
9. L.J. Simpson and M.J. Heben, edited the HS CoE contribution to the DOE 2006 Annual Report
10. M.J. Heben co-organized the “Symposium on Hydrogen Production, Transport, ad Storage” at the Spring meeting of the ECS , Denver CO, May 8-12, 2006.
11. M.J. Heben co-organized and edited the proceedings volume for the “Symposium EE, Hydrogen Storage Materials" at the Spring Meeting of the MRS, San Francisco CA, April 17 -21, 2006.