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

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

Univ Michigan (H₂ spillover and MOFs)

Penn State (B-C-N materials)

Univ North Carolina (nmr)

Duke Univ (Nanocluster seeds)

Rice University (carbon nanotubes, theory)

CalTech (Edge activation, polymers, measurement)

NREL (Materials, theory, measurement, systems, center integration)

Air Products (Materials, measurement, theory, engineering)

NIST (neutrons)

Oak Ridge (Carbon nanohorns)

Livermore (aerogels)

Univ Pennsylvania (polymers)

DOE Annual Merit Review
May 15-18, 2007

This presentation does not contain any proprietary or confidential information
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.
O. Test Protocols and Evaluation Facilities.

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

<table>
<thead>
<tr>
<th>DOE 2010 Technical Targets for Storage System</th>
</tr>
</thead>
<tbody>
<tr>
<td>- Gravimetric 0.06 kg H₂/ kg</td>
</tr>
<tr>
<td>- Volumetric 0.045 kg H₂/m³</td>
</tr>
</tbody>
</table>
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

Area 1: Materials Development
- Air Products: Cooper Activation, complex heterostructures
- Duke: Liu Nanostructured catalysts, templated synthesis
- Caltech: Ahn Engineered dipole structures
- Rice: Tour / Hauge Nanospace management Propped/doped SWNT architectures
- ORNL: Geohegan Carbon nanohorns, metal incorporation

Area 2: Hydrogen Measurements
- LLNL: Satcher, Baumann Metal/carbon aerogels
- U Penn: MacDiarmid Conducting Polymers
- Penn State: Eklund, Foley, Chung B-C-N materials
- U Mich: Yang Hydrogen spillover
- NREL Group Laser, arc, CVD, chemical and gas phase synthesis and processing

Area 3: Predictive Theory
- NREL / Penn State Raman spectroscopy
- NIST: Neumann, Brown Neutron spectroscopy Prompt gamma analysis
- U North Carolina: Wu Nuclear magnetic resonance
- LLNL: Herberg Nuclear magnetic resonance
- Group Analysis Volumetric, gravimetric, TPD
- Penn State: Eklund Caltech: Ahn / Bowman Air Products: Cooper / Pez U Mich: Yang
- NREL: Parilla/Simpson

Area 4: Systems, Analysis & External Connections
- Air Products: Cheng Multi-component systems
- Air Products: Pez Systems Guidance
- Argonne and Systems analysis group
- International Energy Agency IPHE Southwest Research Institute Richard Chahine Additional collaborations
- NREL in-house expertise on vehicle and techno-economic analysis
- Tech Team

- Center is organized into five disciplines
- Collaboration across disciplines speeds development
CoE Accomplishment: Nanospace

Motivation: Enhanced H$_2$ binding with optimized structure

Scaffolded Nanostructures - Rice

C-H$_2$-C theory
Rice, APCI, NREL, +

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

Materials Synthesis

Microporous Carbons - NREL

Measurement & Characterization

Templated Carbons - Duke

Small volumetric & TPD - NREL

Neutron scattering NIST

NMR - UNC

High Accuracy Volumetric - APCI

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 m²/g
    - 1 wt% per 500 m²/gm
    - 3200 m²/gm for 2.1 g/cc material
  - MOF-177: ~7 wt% per 5900 m²/g
    - >2x SSA, but only 40% increase in uptake, 1 wt% per 840 m²/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 m²/g
    - 1 wt% per 390 m²/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

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

Motivation: Enhanced \( H_2 \) binding w/ boron

C-B-H\(_2\) theory
NREL, PSU

B-doped materials - PSU
Carbons and arc SWNTs

B-doped materials - NREL
Laser SWNTs

Materials Synthesis

Future: Increase SSA and B-doping


Kim, et al., PRL 96, 016102 (2006)


Measurement & Characterization

Volumetric - PSU
Neutron scattering - NIST

Small volumetric & TPD - NREL
NMR - UNC

High Accuracy Volumetric - APCI

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 m²/gm vs 2500 m²/gm).
- H₂ uptake at 77K for Chung material is ~50% higher than carbon with same SSA.
- 9.2 kJ/mol H₂ (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 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

C-M-H$_2$ theory
NREL, Rice, PSU, etc.

Y. Zhao CPL 425, 273 (2006)

Materials Synthesis

M-Scaffolding Nanostructures - Rice

M-SWNHs - ORNL

M-Carbons - Duke

M-CA - LLNL

M-BB, SWNTs, Carbons - NREL

Measurement & Characterization

Volumetric - Caltech

Neutron scattering - NIST

Small volumetric & TPD - NREL

NMR - UNC

High Accuracy Volumetric - APCI

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)

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.

Phenomenological spillover schematics

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

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

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

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

CoE Accomplishment: Materials Discovery

- 6.1 wt% Ca$_2$@C$_{60}$H$_{52}$
- 10.5 wt% C$_3$B$_2$ScH$_{12}$
- 8.6 wt % B$_{60}$Sc$_{20}$H$_{144}$
- ~8 wt % (C$_6$N$_2$)$_n^{2n+2nF^-}$, ~20 kJ/mol H$_2$ ads. energy

Rice’s 3-D SWNT foam with nanometer diameter pores and channels (~2600 m$^2$/g) is metallic and may have higher H$_2$ binding due to structure

6.1 wt% Ca$_2$@C$_{60}$H$_{52}$

10.5 wt% C$_3$B$_2$ScH$_{12}$

8.6 wt % B$_{60}$Sc$_{20}$H$_{144}$

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

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• Synthesis and measurement test theoretical approach
• Theory establishes targets for synthesis

NREL  
APCI

PSU  
Rice

New Materials
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.

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

Recommendation

- Recommend No Go

Bulk, as produced SWNTs

- 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
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.
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\textsubscript{2} uptake, up to 8 wt\% possible.
• Partner collaborations have enabled boron doped carbons that bind H\textsubscript{2} at \sim 12 \text{kJ/mol}:
  May enable \sim\text{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 H₂ materials development
  - e.g. H₂ BET surface area measurements that accurately correlate to H₂ 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 H₂ 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
- 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

<table>
<thead>
<tr>
<th>Storage Parameters</th>
<th>Units</th>
<th>System Targets (2010)</th>
<th>MOF-177(^a) (UM/UCLA)</th>
<th>Spillover (UM)</th>
<th>SWNTs (NREL)</th>
<th>M-C(_{60}) (NREL)</th>
<th>Aerogels (LLNL)</th>
<th>Pt-SWNH (ORNL)</th>
<th>Reduced Carbons(^d) (NREL)</th>
<th>B-doped Carbons(^e) (PSU)</th>
</tr>
</thead>
<tbody>
<tr>
<td>FY05</td>
<td>FY06</td>
<td>FY05</td>
<td>FY06</td>
<td>FY05</td>
<td>FY06</td>
<td>FY06</td>
<td>FY07</td>
<td>FY07</td>
<td>FY07</td>
<td>FY07</td>
</tr>
<tr>
<td>Specific Energy</td>
<td>Wt% H(_2)</td>
<td>6</td>
<td>2.5</td>
<td>7</td>
<td>1.6</td>
<td>b</td>
<td>3</td>
<td>0.5</td>
<td>0.5</td>
<td>4.2</td>
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<tr>
<td>Volumetric Energy</td>
<td>g/L</td>
<td>45</td>
<td>*</td>
<td>31</td>
<td>*</td>
<td>41</td>
<td>*</td>
<td>28</td>
<td>*</td>
<td>29</td>
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<td>Capacity</td>
<td></td>
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</tbody>
</table>

|                   | 77 K, 50 bar | 77 K, 60 bar | RT, 100 bar | RT, 100 bar | 77 K, 20 bar | STP | 77 K, 30 bar | STP | 77 K, 30 bar | STP | 77 K, 30 bar | STP |
|                   | 77 K, 20 bar | 77 K, 30 bar | STP | 10 Bar | 77 K, 30 bar | STP | 77 K, 30 bar | STP | 77 K, 30 bar | STP | 77 K, 30 bar | STP |

* Information not available
  Volumetric capacities derived from material densities
  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 LiBH\(_4\), 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 m\(^2\)/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

<table>
<thead>
<tr>
<th>Storage Parameters</th>
<th>Units</th>
<th>System Targets (2010)</th>
<th>Organometallic Fullerenes (^a) (NREL)</th>
<th>MetCars (^b) (NREL)</th>
<th>Macro-molecules (NREL)</th>
<th>Endohedral Metallofullerene (^c) (NREL)</th>
<th>Metallo-carborane (^d) ((C_6N_2)_n) (2nF^-) (APCI)</th>
<th>Spillover on SWNT (NREL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>FY05</td>
<td>FY06</td>
<td>FY06</td>
<td>FY07</td>
<td>FY07</td>
<td>FY07</td>
<td>FY07</td>
<td>FY07</td>
<td>FY07</td>
</tr>
<tr>
<td>Specific Energy</td>
<td>Wt% H(_2)</td>
<td>6</td>
<td>~9</td>
<td>3.7-7.7</td>
<td>&gt;5</td>
<td>6.1</td>
<td>10.5</td>
<td>7.4(^e)</td>
</tr>
<tr>
<td>Volumetric Energy Capacity</td>
<td>g/L</td>
<td>45</td>
<td>52-43</td>
<td>48-58</td>
<td>&gt;40</td>
<td>*</td>
<td>52</td>
<td>*</td>
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<tr>
<td>Comments</td>
<td></td>
<td></td>
<td>STP, 23-46 (\text{kJ/mol})</td>
<td>STP, 15-32 (\text{kJ/mol})</td>
<td>STP</td>
<td>~STP, 10-78 (\text{kJ/mol})</td>
<td>STP</td>
<td>~STP, ~20 (\text{kJ/mol})</td>
</tr>
</tbody>
</table>

* Information not available

Volumetric capacities derived from material densities
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

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.
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 Engrtrakul (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.
13. “University of North Carolina 1H NMR study of ORNL SWNH Materials.” Primary contacts: Hui Hu (ORNL) and Alfred Kleinhampes (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.
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 Kleinhampes, 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).
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 Kleinhannmes (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.


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.


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

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 LiBH₄ or MgH₂.
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 NaAlH₄ 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 scaffates.
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.
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.
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.
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 (YTA 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.
29. University of Colorado. NREL assisted Rishi Raj in developing a CU program on H₂ storage using polymer derived ceramics (Raj, Heben).
Anne Dillon is leading the organization of a session entitled "The Hydrogen Economy" at the spring 2008 MRS meeting in San Francisco.

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.

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.

M.J. Heben co-organized a session on “Hydrogen Production, Transport, and Storage 2” at the ECS meeting in Chicago (May 6 -11, 2007).

M.J. Heben co-organized a symposium at the MRS Fall meeting, Boston, MA, in November 2006.

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.

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.


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.

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.