

IV.C.1a NREL Research as Part of the Hydrogen Sorption Center of Excellence

Michael Heben (Primary Contact), J.L. Alleman, J.L. Blackburn, C. Curtis, A.C. Dillon, C. Engtrakul, T. Gennett, K.M. Jones, Y.-H. Kim, K.J. O'Neill, P.A. Parilla, L.J. Simpson, E. Whitney, Y. Yan, S.B. Zhang, Y. Zhao
National Renewable Energy Laboratory (NREL)
1617 Cole Blvd.
Golden, CO 80401
Phone: (303) 384-6641; Fax: (303) 384-6655
E-mail: michael_heben@nrel.gov

DOE Technology Development Manager:
Carole Read
Phone: (202) 586-3152; Fax: (202) 586-9811
E-mail: Carole.Read@ee.doe.gov

Subcontractor:
Rochester Institute of Technology, Rochester, NY

Project Start Date: FY 2005
Project End Date: Project continuation and direction determined annually by DOE

Objectives

NREL is performing research and development (R&D) and coordinating the Hydrogen Sorption Center of Excellence (HSCoE) to develop the science base and technology advances required to meet DOE's on-vehicle hydrogen storage targets. FY 2007 research efforts were focused on:

- Using theory as a guide, actively pursued the synthesis of new promising compounds for reversible hydrogen storage with desired binding energies.
- Determining structures of new compounds and correlating the structures with adsorption mechanisms, desired binding energies and capacities (volumetric and gravimetric).
- Employing theory to explain and confirm observed experimental results as well as establishing optimized structures that have rational synthesis routes.
- Expanding hydrogen capacity measurement capabilities for rapid screening to improve round robin process/sample exchange with partners.
- Continuing theoretical efforts to predict/design new sorption materials consisting of light elements but not restricted to a carbon base.

Technical Barriers

The technical barriers address by this project from the Hydrogen Storage section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan, include:

- (A) System Weight and Volume
- (B) System Cost
- (C) Efficiency
- (D) Durability/Operability
- (E) Charging/Discharging Rates
- (J) Thermal Management
- (P) Lack of Understanding of Hydrogen Physisorption and Chemisorption
- (Q) Reproducibility of Performance

Technical Targets

This effort is focused on the development of materials that can meet DOE hydrogen storage system targets (e.g. 0.06 kg H₂/kg and 0.045 kg H₂/m³). Lists of representative experimental results and theoretical predictions are provided in Table 1 and 2, respectively.

Accomplishments

- Developed, through rational design, several new hydrogen storage materials with unique hydrogen sorption sites and properties:
 - Synthesized six novel organometallic fullerene compounds, each with unique hydrogen adsorption sites, using scalable processing. Structural characterization as well as H₂ capacity measurements suggests that these materials warrant further study.
 - A new hydrogen adsorption mechanism was revealed on Na⁺ reduced (hydrogenated) carbon materials. These materials demonstrate ~5 wt% hydrogen storage at ambient conditions and release the hydrogen at relatively low energies compared to typical hydride or chemically bonded hydrocarbons.
 - Both arc and laser-generated B-doped single-walled nanotubes (SWNTs) have been made and evaluated with neutron scattering (~2 at% B-loading). While this low boron content is too small to significantly affect hydrogen

TABLE 1. Progress Towards Meeting Technical Targets for Hydrogen Storage for Transportation Applications: Synthetic Results

Material Performance													
Storage Parameters	Units	System Targets (2010)	SWNTs, validated ^a	B-SWNT		Fe(C ₆₀)		Cr(C ₆₀)	Li(C ₆₀)	Reduced SWNTs		Reduced AX-21	<4 Angstrom Pore Size Material
			FY 2006	FY 2005	FY 2006	FY 2006	FY 2007	FY 2007	FY 2007	FY 2006	FY 2007	FY 2007	FY 2007
Specific Energy	wt% H ₂	6	3	*	~2.2 ^b	0.5	1	0.5	0.5 ^c	4 ^d	4 ^d	5 ^d	1.5
Volumetric Energy Capacity	g/L	45	28	*	20	*	*	*	*	37	37	*	*
Comments			77 K, 20 bar		77 K, 20 bar	77 K, 2 bar	77 K, 85 bar	77 K, 2 bar	STP ^e	STP ^e	STP ^e	STP ^e	77 K, 2 bar

* Information not available

Volumetric capacities derived from material densities

a. 3 wt% results reproduced at different laboratories.

b. Blackburn et al. Chem. Mat. 18 2558 (2006), B-doping level (~1-2% now) will be increased as precursors / techniques develop.

c. When excess Li is present.

d. Mostly irreversible. Demonstrates potential reversible capacity once dissociation material can be incorporated with lattice.

e. STP - Standard temperature and pressure.

TABLE 2. Progress Towards Meeting Technical Targets for Hydrogen Storage for Transportation Applications: Predicted Materials

NREL Theoretical Materials Predictions									
Storage Parameters	Units	System Targets (2010)	Organo-metallic Fullerenes ^a	MetCars ^b	Macro-molecules	Endohedral Metallo-fullerene ^c	Metalla-borane	C ₃ B ₂ Sch ₁₂	Spillover on SWNT
			FY 2005	FY 2006	FY 2006	FY 2007	FY 2007	FY 2007	FY 2007
Specific Energy	wt% H ₂	6	~9	3.7-7.7	>5	6.1	8.6	10.5	>7.7
Volumetric Energy Capacity	g/L	45	52-43	48-58	>40	*	52	52	~56
Comments			STP, 23-46 kJ/mol	STP, 15-32 kJ/mol	STP	~STP, 10-78 kJ/mol	STP	STP	RT ^d , 100 bar

* Information not available

Volumetric capacities derived from material densities

a. Zhao et al. PRL 94, 15504 (2005).

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

c. Y. Zhao et al. submitted

d. RT - room temperature

storage capacities, enhanced binding energies (10–12 kJ/mol) have been demonstrated.

- Designed and identified through computation new classes of hydrogen storage materials that have the potential to meet DOE targets.
 - Performed local density approximation calculations that indicated enhanced hydrogen

binding occurs with higher B concentration and curvature. Increased curvature of B-doped carbon enhances hydrogen binding by nearly 50%. Furthermore, the calculations indicate that B prefers defect/kinked sites and in these sites have higher hydrogen binding energies.

- Performed investigations to identify new systems with over 6 wt% hydrogen storage, including:
 - Metallaboranes ($B_{60}Sc_{20}H_{144}$) ~8.6 wt%, reversible, 52 kgH₂/m³
 - Metallacarboranes ($C_3B_2TiH_{11}$) ~8.6 wt%, reversible, 43 kgH₂/m³
 - $C_3B_2ScH_{12}$: ~10.5 wt%, reversible
- Endohedral metallofullerenes (e.g. Ca₂@C₆₀H₅₂) 6.1 wt%, reversible, ~50 kg/m³.
- Identified that transition metal boride nanoparticles have stable high surface area cage structures suitable for reversible high capacity hydrogen storage at near ambient conditions.
 - Transition metal-boride cages (M4B12, M8B12, M12B16, and M12B20, where the M can be any 3d transition metal [TM] atoms) are a new class of stable materials that should have good hydrogen storage properties.
 - ScB₃ nanotubes were identified to be highly stable and to have dihydrogen binding energies around 20 kJ/mol.
- Identified that splitting and occupation of spin orbitals in metal organic framework (MOF) systems may account for their unexpectedly smaller binding energies. NREL calculations exactly describe the observed binding energy for the Mn₂₊-exposed MOF system (i.e. ~10 kJ/mol). NREL also identified that the dihydrogen binding energy can be tuned between 10 and 50 kJ/mol by using other early TM elements. This effort demonstrates how computational analysis is necessary to accurately determine specific binding mechanisms and to define paths for improved storage.
- Determined that there exists optimal metal-metal distances to achieve maximum hydrogen capacity; resolve metal clustering issues; and to determine that metal atoms stabilize heavily doped carbon cages or nanotubes.
- Hydrogen measurement capabilities have been improved to accelerate development of materials that can meet DOE storage targets. This includes volumetric, pore size, and surface area measurements with variable temperature control and high-pressure spectroscopies at temperatures from 77 to ~300 K on laboratory size samples (1-5 mg).
- Performed and completed characterization and hydrogen storage capacity measurements on materials sent to NREL from various HSCoE partners as well as with other collaborators outside the HSCoE. This included providing hydrogen

storage related characterization results involving >200 individual measurements from >50 different samples, in collaboration with ~20 institutions.



Introduction

NREL leads the HSCoE to develop reversible sorbent materials for hydrogen storage within the U.S. DOE National Hydrogen Storage Program. The NREL effort is based on coupling capacity, binding energy, material structure, and mechanistic measurements with novel synthetic techniques and advanced theoretical studies to rationally identify and develop new materials that address the storage barriers delineated in DOE's Multi-Year RD&D Plan. The interplay between these efforts elucidate the physics and chemistry of uptake and enable the design of new materials with superior performance. During the past year, NREL has worked with a wide array of promising nanostructured materials, and developed new adaptable, repeatable, and potentially scalable synthesis strategies. Hydrogen storage capacities of the nanostructured adsorbent materials of interest are accurately measured with custom-built temperature programmed desorption and volumetric apparatuses. The capacity measurements support materials development work being done in-house and at HSCoE partners, and are also used to analyze promising samples prepared by researchers from other collaborating institutions. A thorough understanding of the sources of error in hydrogen storage measurements has permitted simplification of the measurement processes, allowing the development of high throughput methods. Advances are disseminated to HSCoE partners and the larger hydrogen storage community and will help to establish standard test protocols for evaluating reversible hydrogen storage materials.

Approach

NREL focuses on accelerating the rational synthesis of multiple compounds that are promising for meeting DOE on-vehicle hydrogen storage system targets. An emphasis is placed on finding structures with desirable binding energies along with optimized surface area and site density. The synthetic development employs both wet chemical and gas phase processes to generate new hydrogen sorption materials. For example, wet chemical routes are developed to synthesize the organometallic fullerenes structures designed by Zhao et al. PRL 94 155504 (2005). In addition, gas phase processes are developed to generate boron-doped (e.g. designed by Kim et al. PRL 96 016102 (2006)) and other novel hydrogen storage materials. Once new materials are developed, their performance is compared

to the theoretical predictions to provide feedback to the modelers and enable development of new material designs. Furthermore, first principle models are developed to identify potential synthesis pathways and identify other novel materials. All this materials design and synthetic effort is complemented by development of high throughput measurement capabilities for laboratory scale samples to accelerate discovery, development and partner interactions.

Results

Hydrogen Storage Materials Design

As part of NREL's rational design of hydrogen storage materials, we performed first-principles studies using density functional theory. These calculations are used to predict the minimum energy structures, reaction pathways, electronic properties, and, in particular, the binding characteristics of the various forms of hydrogen to the storage hosts. As part of this effort NREL also coordinated theoretical and computational efforts occurring throughout the center. Specific NREL development efforts included:

- Identifying additional new carbon-based systems in which Kubas-type interactions can significantly increase the volumetric storage density to above the 6 wt% DOE system target. A class of materials termed metallocarboranes $C_{36}B_{24}Ti_{12}$ and $C_{36}B_{24}Sc_{12}$ were designed with reversible hydrogen storage of $\sim 8.6\%$ wt% ($43 \text{ kg H}_2/\text{m}^3$) and $\sim 10.5 \text{ wt}\%$, respectively. In addition, a new class of metalloboranes (e.g. $B_{60}Sc_{204}$) were designed with up to 8.6% wt% ($52 \text{ kg H}_2/\text{m}^3$) reversible hydrogen storage. Finally, a group of endohedral metallofullerenes were identified (e.g. $Ca_2@C_{60}H_{52}$, Figure 1) with up to 6.1% wt% ($50 \text{ kg H}_2/\text{m}^3$) reversible hydrogen storage. The specific details associated with these findings will be published in the near future.
- Based on first principle calculations, NREL identified a new class of potential hydrogen storage material involving four types of stable transition metal-boride cages (M4B12, M8B12, M12B16, and M12B20, where the M can be any 3d TM atoms). As an example, the M8B12, with the identical topology as the Ti_8C_{12} (metcar) molecule that have been synthesized, are only stable with Cr, Mn, Fe, and Co.
- NREL computations identified that two types of ScB3 nanotubes may be potential hydrogen storage materials. However, the Sc-coating structure are less stable than the Sc-embedded ones. The Sc-embedded nanotube is $0.8 \text{ eV}/(\text{ScB}_3)$ lower than the Sc-coating nanotube. At small-diameter, the Sc-embedded nanotube is semiconducting, but the Sc-coating nanotubes are always metallic. Preliminary

calculations indicate that the Sc atoms in the novel nanotubes can store dihydrogen with a binding energy around 20 kJ/mol .

- Calculations determined the existence of optimal metal-metal distances to achieve the maximum hydrogen capacity on a given framework. In addition, thermodynamic and kinetic considerations were used to resolve metal clustering issues and to determine that metal atoms can be used to stabilize heavily doped carbon cages or carbon nanotubes.
- Enhanced hydrogen binding was found to occur with higher B concentrations and curvature of graphene structures. These investigations systematically identified the affect of increased curvature of B doped carbon and determined that the binding can be enhanced by nearly 50% with highly curved structures like small diameter single walled nanotubes or fullerenes. Furthermore, the calculations indicated that B prefers defect/kinked sites and in these sites the boron has even higher hydrogen binding than as a dopant in a graphene layer.
- Identified systems in which both the carbon-hydrogen bond strength and the H diffusion barrier are optimal for spillover to take place. This involved developing an atomistic model of spillover with three key elements: (i) the driving force for the H to leave its gas phase to be stored, (ii) low-energy-barrier diffusion pathways on the storage materials, and (iii) the lack of ability for the H to desorb as H_2 before reaching its final destination. Specific components of this work have been submitted for publication.

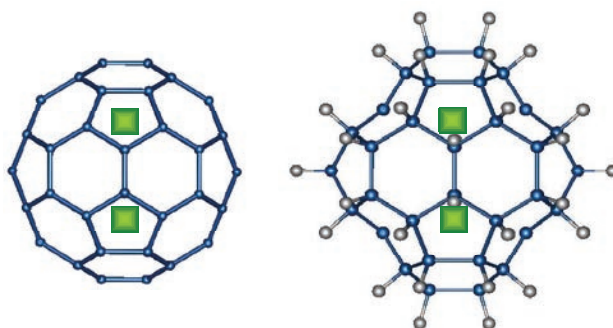


FIGURE 1. Endohedral metallofullerenes have recently been proposed for hydrogen storage by H. Dorn at Virginia Tech. Collaborating with Professor Dorn, NREL performed calculations to determine their hydrogen storage characteristics. NREL calculations indicate that Ca_2 is the optimal endohedral dopant for hydrogen storage via hydrogenation. Similar endohedral fullerenes have been easily synthesized at high yield; e.g. *Ge et al. JACS 127 (2005) 16292*. Charge transfer from Ca_2 allows for both reversible hydrogen storage as well as the stabilization of negative curvature in the fullerene. A paper by Zhao et al. has been submitted for publication.

Synthesis of Nanostructured Sorbents

Synthesis of novel nanostructured sorbents with high hydrogen storage capacities is essential to demonstrate that sorption-based materials may meet the DOE system targets and to provide feedback for additional materials discovery. Thus, NREL continued to explore and quantify the potential of solution- and gas-phase chemistry to synthesize sorption-based complexes that stabilize molecular hydrogen ligands (dihydrogen) or enable other forms of hydrogen storage. These efforts included:

- Doped or intercalated sp^2 -hybridized carbon nanostructures as well as new alternative molecules were developed to investigate their hydrogen storage properties. One synthesis route involved substitution reactions on C_{60} - M_x species. This led to the development of six distinctly different metallofullerene complexes where complexed metals (Li, K, Sc, Cr, Co, and Fe) were used to stabilize dihydrogen ligands and increase the H_2 capacity. Each material demonstrated unique hydrogen storage properties, higher capacities than the base fullerene material, and higher binding energies (Figure 2). Thus, the initial results are very promising and indicate that additional work should be performed to optimize metal loading at specific sites and to create nanostructures with enhanced hydrogen storage properties.

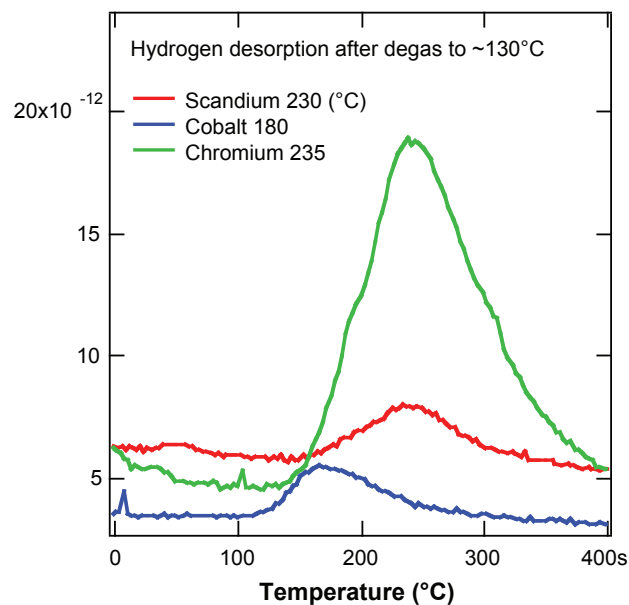


FIGURE 2. Temperature-Programmed Desorption of $Cr(C_{60})$, $Sc(C_{60})$, and $Co(C_{60})$ compounds indicate higher hydrogen binding energies. The metal decorated fullerenes typically have higher storage capacities, compared to fullerenes alone, with up to 0.5 wt% demonstrated at ambient conditions.

- Reduction of carbon materials (e.g. SWNTs or activated carbon) using sodium-containing solvents results in the hydrogenation of the carbon surfaces. Typical carbon hydrides have very strong binding energies that requires temperatures in excess of $600^\circ C$ to liberate the hydrogen. However, the sodium reduced hydrogenated carbons begins releasing hydrogen at $\sim 100^\circ C$ and releases all of the hydrogen below $500^\circ C$ (Figure 3). Detailed studies with deuterium indicated that the hydrogen is being provided by a chemical breakdown of the solvent. Thus a new hydrogenation route and a new hydrogen storage mechanism have been demonstrated. Initial investigations demonstrated ~ 5 wt% hydrogen storage at ambient conditions and release of the hydrogen at relatively low energies compared to typical hydride or chemically bonded hydrocarbons. These efforts have important implications for improved kinetic and thermodynamic reversible storage involving hydrogenation (e.g. spillover). Future efforts will optimize the storage capacity and binding energy to develop materials that can meet DOE hydrogen storage targets.
- B-doped SWNTs were generated from arc and laser based processes. These materials were evaluated in detail with standard hydrogen storage measurements, nuclear magnetic resonance, and neutron scattering. Neutron scattering and X-ray dispersive spectroscopy indicated that the materials had $\sim 2\%$ B-loading. While this low boron content is too small to significantly affect hydrogen storage capacities, enhanced binding ($10\text{--}12$ kJ/mol) and

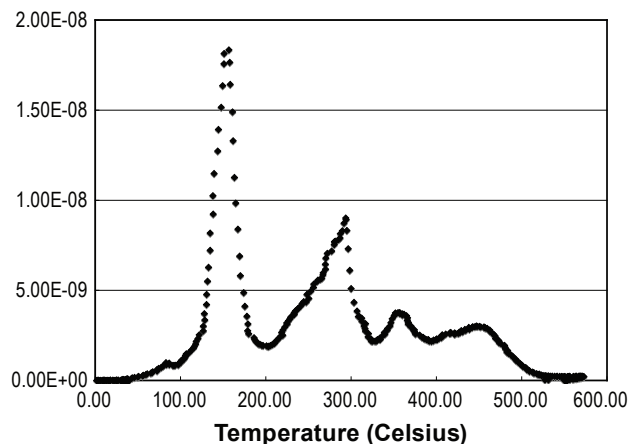


FIGURE 3. A new reduction process using sodium results in an unique hydrogenation of carbon materials. The hydrogenation of AX-21 results in ~ 5 wt% storage and release of all the hydrogen below $500^\circ C$, while most is released below $300^\circ C$. Hydrogenation of typical carbon materials using other processes generally requires temperatures in excess of $600^\circ C$ to liberate the hydrogen. This approach comments on key aspects of spillover.

- other significant material property improvements were demonstrated. Enhance boron loading will be achieved through the use of boron contain precursors and/or the use of reactive boron containing species in the synthesis processes.
- Developed multiple processes using laser vaporization, chemical vapor deposition, and chemical techniques to form carbon-metal-hydrogen (C:M:H) systems. Metals included Rh, Co, Ni, Cr, Ti, Sc, Pt, and Pd. Purification and hydrogen activation processes were also developed and unique hydrogen storage properties of these materials were demonstrated. For example, spillover was induced using Pt decorated activated carbons and single walled nanotubes. In addition, higher dihydrogen binding energies were demonstrated using Rh decorated SWNTs. Future work will investigate the formation of these and other metals in more specific sites and with the correct hydrogen complexation.

Hydrogen Adsorption Measurements

NREL employs a number of techniques to evaluate the hydrogen adsorption capacities, kinetics, thermodynamics, and pressure/temperature/adsorption behavior of adsorbent samples. In the effort to develop improved hydrogen storage capacities on sorbent materials, many types of novel materials are being synthesized, initially only in small quantities. To measure the hydrogen capacity of these samples in a quick and facile manner, to provide rapid feedback for synthetic optimization, and to address issues such as stability and cyclability of the materials being produced, NREL has focused on developing measurement capabilities that are highly accurate for small samples (less than 5 mg). Most recently, NREL has continued to enhance capabilities to perform high throughput screening measurements on small samples at different temperatures and pressures. These efforts allow detailed studies to be performed to examine the different binding mechanisms used for hydrogen storage.

Conclusions and Future Directions

The rational design and synthesis of enhanced hydrogen storage materials with appropriate binding energies has led to the discovery of new materials with unique and improved properties. This combined with NREL's emphasis on rapid throughput screening of materials has accelerated hydrogen storage materials development and substantially enhanced our understanding of mechanisms that will be needed to meet DOE targets. While NREL continues to investigate the intrinsic properties needed for hydrogen storage, we also developed processing to create several carbon-metal-hydrogen structures and demonstrated their potential to provide enhanced hydrogen storage. Future efforts will include:

- Synthesizing materials with enhanced hydrogen storage properties. This will involve both wet and gas-phase processing and purification of materials that have hydrogen sorption sites with appropriate binding energies arrayed in a matrix for optimal storage capacity at near ambient conditions. In addition, to develop a more complete understanding of the synthetic approaches that may be possible, model or simpler systems will also be explored.
- Continuing to theoretically probe promising new materials including hybrid structures, intercalated graphite as well as non-carbon-based adsorbents. Also, NREL will merge theoretical and experimental efforts such that theory will guide in the synthesis of promising compounds.
- Continuing development of rapid throughput hydrogen storage capacity measurements and the evaluation of partner samples.

Special Recognitions & Awards/Patents Issued

1. "Metal-doped single-walled carbon nanotubes and production thereof," A. C. Dillon, M. J. Heben, T. Gennett, P. A. Parilla, PCT Patent WO03/085178.

Special 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 leads is an International Energy Agency Expert in Annex 22.
7. M.J. Heben is on the organizing committee for a DOE sponsored workshop on "Computational Research Needs in Alternative & Renewable Energy", September, 19–20 2007.

FY 2007 Publications/Presentations

Publications

1. "Sorption Materials for Hydrogen Storage", J.L. Blackburn, A.C. Dillon, C. Engtrakul, Y.H.-. Kim, P.A. Parilla, L.J. Simpson, E. Whitney, S.B. Zhang, Y. Zhao, and M.J. Heben, Chemical Reviews, submitted (2007).

2. “Smart-material Behavior for Endohedral Metallofullerenes in Hydrogen Storage,” Y. Zhao, M. J. Heben, A. C. Dillon, L. Simpson, J. Blackburn, H. C. Dorn, S. B. Zhang accepted by Journal of Physical Chemistry.
3. “Novel Organometallic Fullerene Complexes for Vehicular Hydrogen Storage,” A.C. Dillon, E. Whitney, C. Engtrakul, C. J. Curtis, K.J. O’Neill, P.A. Parilla, L.J. Simpson, M.J. Heben, Y. Zhao, Y-H. Kim and S. B. Zhang (in press) Phys. Stat. Sol. (2007).
4. “Hydrogen storage in carbon-based materials” P. Bénard, R. Chahine, P.A. Chandonia, D. Cossement, G. Dorval-Douville, L. Lafi, and E. Poirier, J.L. Blackburn, C. Curtis, A.C. Dillon, T. Gennett, M.J. Heben, Y.-H. Kim, P.A. Parilla, L.J. Simpson, E.S. Whitney, S.B. Zhang, and Y. Zhao, Final report for Task C1 for the International Energy Agency Hydrogen Implementing Agreement, Task 17, Final Report, 2007.
5. “Measurement of the Reversible Hydrogen Storage Capacity of milligram Ti-6Al-4V alloy samples with Temperature Programmed Desorption and Volumetric Techniques,” Jeff L. Blackburn, Philip A. Parilla, Thomas Gennett*, Katherine E. Hurst, Anne C. Dillon, Michael J. Heben, Journal of Alloys and Compounds, Published online January 5 (2007).
6. “Effects of Surfactant and Boron Doping on the BWF Feature in the Raman Spectrum of Single-wall Carbon Nanotube Aqueous Dispersions,” Blackburn, J. L., Engtrakul, C., McDonald, T., Dillon, A. C., and Heben, M. J., Journal of Physical Chemistry, 110, 25551 (2006).
7. “Inelastic Neutron Scattering of H₂ Adsorbed on Boron Substituted SWNTs,” Y. Liu, C. M. Brown, J. L. Blackburn, D. A. Neumann, T. Gennett, L. J. Simpson, P. A. Parilla, A. C. Dillon, M. J. Heben, Journal of Alloys and Compounds, Special Issue, MH2006.9.
8. “Non-dissociative adsorption of H₂ molecules in light-element doped fullerenes”, Y.-H. Kim, Y. Zhao, A. Williamson, M.J. Heben, and S. B. Zhang, Physical Review Letters 96, 016102 (2006).
9. “Self-catalyzed Hydrogenation and Dihydrogen Adsorption on titanium carbide nanoparticles” Y. Zhao, A. C. Dillon, Y.-H. Kim, M. J. Heben, and S. B. Zhang, Chem. Phys. Lett. 425, 273 (2006).
10. “Synthesis and Characterization of Boron-doped Single-wall Carbon Nanotubes Produced by the Laser Vaporization Technique”, Jeff L. Blackburn, Yanfa Yan, Chaiwat Engtrakul, Philip A. Parilla, Kim Jones, Thomas Gennett, Anne C. Dillon, Michael J. Heben. Chemistry of Materials 18(10), 2558 2006.
11. “Hydrogen Storage in Novel Carbon-based Nanostructured Materials,” E.S. Whitney, C.J. Curtis, C. Engtrakul, M.R. Davis, T. Su, P.A. Parilla, L.J. Simpson, J.L. Blackburn, Y. Zhao, Y-H. Kim, S.B. Zhang, M.J. Heben and A.C. Dillon Mat. Res. Soc. Proc., Fall 2006.
12. “High Throughput, High Purity Single Wall Carbon nanotube Synthesis in a Volumetric Confined Arc Chamber,” T. Gennett, C. Engtrakul, K. J. Franz, J. A. Alleman, P. A. Parilla, K.M. Jones, J. Blackburn, K. E. H. Gilbert, Jamie Ellis, A. C. Dillon, M. Heben, manuscript in preparation.
13. “Alkali-Metal Induced Hydrogenation Reactions of Single Wall Carbon Nanotubes,” T. Gennett, C. Engtrakul, C. Curtis, J.E. Ellis, L.J. Simpson, J. Blackburn, A. Dillon, M. Heben., manuscript in preparation.
14. “Rapid, accurate, in situ, calibration of a mass spectrometer for temperature programmed desorption studies”, K.E.H. Gilbert, P.A. Parilla, J.L. Blackburn, T. Gennett, A.C. Dillon, and M.J. Heben, manuscript in preparation.
15. “Competitive adsorption between carbon dioxide and methane on carbon nanotube materials” K.E.H. Gilbert, P.A. Parilla, J.L. Blackburn, T. Gennett, A.C. Dillon, and M.J. Heben, manuscript in preparation.

Invited Presentations

1. “DOE Carbon CoE Overview,” M. Heben (invited talk) DOE Annual Merit Review, Alexandria, VA, May 15–18, 2007.
2. “NREL Research as Part of the Carbon CoE,” A. Dillon (invited talk) DOE Annual Merit Review, Alexandria, VA, May 15–18, 2007.
3. “DOE Carbon-based Hydrogen Storage CoE Overview,” L. J. Simpson (invited poster) DOE Annual Merit Review, Alexandria, VA, May 15–18, 2007.
4. “Nanoscience for Energy Conversion and Storage” M.J. Heben, University of Maryland, University of Maryland Energy Research Center Colloquium, April 23, 2007.
5. “Nanoscience for Energy Conversion and Storage,” M.J. Heben, Colorado School of Mines, Chemistry Department Colloquium, April 12, 2007.
6. “First-Principles Materials Theory: The Promises and Challenges”, Shengbai Zhang, Colloquium, Department of Physics and Astronomy, Washington State University, Pullman, April 5, 2007.
7. “Nanoscience for Energy Conversion and Storage” M.J. Heben, University of Toledo, Department of Physics and Astronomy Colloquium, April 2, 2007.
8. “Group IV Clusters: New Symmetry and Novel Storage Materials”, Shengbai Zhang, Colloquium, Depart. of Chem., U. of Nebraska, Lincoln, March 23, 2007.
9. “Novel Organometallic Fullerene Complexes for Vehicular Hydrogen Storage” A. C. Dillon (invited) International Winter School on Electronic Properties of Novel Materials, Kirschberg, Austria, March 14, (2007).
10. “Theory for hydrogen storage: the organometallic approaches” Yufeng Zhao, (invited Colloquium) Dept. Physics, Colo. Sch. of Mines, Golden, CO, Jan. 16, (2007).

11. “First-principles study of nanostructured materials for room-temperature reversible hydrogen storage,” Shenbai Zhang (invited talk and also session chair) International Workshop on “Clusters - A Bridge Across Disciplines” on Jekyll Island, Georgia, Dec. 16-20, 2006.
12. “Update on activities for NREL’s Hydrogen Storage Research Program,” Phil Parilla, (invited talk and panelist) Storage Systems Analysis Working Group (SSAWG), Washington, D.C., 12/12/06.
13. “On the Road to Viable Hydrogen Storage Systems,” Mike Heben (invited talk and session chair) Boston, MA, Fall 2006 MRS conference.
5. “Smart-Material Behavior for Endohedral Metallofullerenes in Hydrogen Storage” Yufeng Zhao, M. J. Heben, A. C. Dillion, L. Simpson, J. L. Blackburn, H. C. Dorn, and S. B. Zhang, (contributed talk), APS March Meeting, Denver, CO March 2007.
6. “Hydrogen Storage in Novel Carbon-based Nanostructures: Fe-C60,” Erin Whitney (contributed talk) Gordon Conference on Renewable Fuels in Ventura Beach, California, Jan. 21-26, 2007.
7. “Hydrogen Storage in Novel Organometallic Fullerene Complexes,” Erin Whitney (contributed talk) Fall MRS Conf., Boston, MA, Nov. 2006.

Contributed Presentations

1. “Hydrogen Storage Materials Investigations of Nanostructured Sorbents,” L.J. Simpson, P. Parilla, J. Blackburn, K. O’Neill, T. Gennett, C. Engtrakul, E. Whitney, A. Dillon and M. Heben, (contributed talk) Electrochemical Society Conference, Chicago, IL, May 5–11 (2007).
2. “Alkali Metal Reduced Carbon Single- Walled Nanotubes as Primary Hydrogen Storage Materials,” T. Gennett, C. Curtis, C. Engtrakul, J. Ellis and M. Heben (contributed talk) Electrochemical Society International Meeting, Chicago, Illinois, May 2007.
3. “Novel H₂ Sorption Measurements of Nanostructured Materials,” L.J. Simpson, P. Parilla, J. Blackburn, K. O’Neill, T. Gennett, C. Engtrakul, E. Whitney, A. Dillon and M. Heben, (contributed talk) American Physical Society, Denver, CO March 5-9 (2007).
4. “High Pressure Volumetric Sorption Measurements On Small Samples At Low Temperatures”, P. A. Parilla, L.J Simpson, J.L. Blackburn, A.C. Dillon, and M.J. Heben, (contributed talk), March APS Meeting, Denver, CO, March 2007.
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