IV.C.7 H$_2$ Storage Characterization and Optimization Research Efforts

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Project Start Date: October 1, 2015
Project End Date: Project continuation and direction
determined annually by DOE

Overall Objectives

- Develop a series of advanced characterization tools that allows for rapid advancement and in-depth understanding of next-generation hydrogen storage materials.

- Develop a hydrogen storage material with a total materials-based capacity of >45 g/L above 150 K, that is possible with hydrogen overpressures <100 bar and reversible for multiple cycles.

- Optimize thermal management in hydrogen storage systems by the incorporation of unique phase-change materials.

- Demonstrate the importance of computational methods in developing and understanding of next generation hydrogen storage materials.

Fiscal Year (FY) 2016 Objectives

- Develop new characterization tools (specifically thermal conductivity, nuclear magnetic resonance [NMR], Fourier transform infrared).

- Demonstrate the ability to bind two H$_2$ molecules to one metal center in a metal-organic framework, porous aromatic framework, or carbon-based material.

- Demonstrate the ability to increase the binding energy in high surface area carbon-based sorbents.

- Demonstrate the ability to control binding energies in sorbent materials.

- Develop computational methodologies for predicting hydrogen storage properties in sorbents with unsaturated metal centers.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan.

General

(A) System Weight and Volume

(B) System Cost

(C) Efficiency (Refueling Time)

Reversible Solid-State Material

(O) Lack of Understanding of Hydrogen Physisorption and Chemisorption(P) Reproducibility of Performance

Technical Targets

Hydrogen Storage Materials:

This project is conducting validation studies of various framework materials, sorbents, hydrides, and model compounds. Concurrently, the team also is developing new characterization tools for the rapid enhancement of materials development. Insights gained from these studies will be applied toward the design and synthesis of hydrogen

storage materials that meet the following DOE onboard 2020 automotive hydrogen storage targets.

- 1.8 kWh/kg system (5.5 wt% hydrogen)
- 1.3 kWh/L system (0.040 kg hydrogen/L)
- Cost of \$10/kWh (\$333/kg H_2 stored).
- An onboard efficiency of 90% and minimum delivery pressure of 3 bar
- Total refuel time of 5 min

FY 2016 Accomplishments

- Observed and verified the binding of two hydrogen molecules to an unsaturated metal center within a metal organic framework material.
  - Established through neutron diffraction and inelastic scattering spectroscopy.
  - Developed NMR methods to validate 2 H_2/metal site in an amorphous material.
- Established control of desorption temperatures with the molecular hydrogen in model oxocarbon species by changing the metal centers for a final range from 80 K to 300 K.
- Established the ability to modify carbon sorbents with the introduction of unsaturated metal sites with overall increasing desorption temperature from 80 K to 110 K.
- Enhanced the kinetics of hydrogen interaction with borohydride materials.
  - Validated key additives to increase the rate of H_2 uptake and release in BH_4/$B_{10}H_{10}$ cycle.
  - Demonstrated the regeneration of borohydride from closo-decaborane.
- Developed a one-of-a-kind thermal conductivity apparatus that can operate from 50–380 K with gas overpressures up to 100 bar.
- Developed advanced porous aromatic framework materials with >1,000 m^2/gram surface area.
- Designed and ordered a state-of-the-art in situ infrared spectrometer for measuring spectra in H_2-dosed materials.
- Established the capacities of multiple external laboratory materials under investigation for DOE.
- Established a consensus with DOE, tech team, and international partners as to protocols for reporting volumetric capacity of sorbent materials.
- Established multiple experimental and modeling partnerships and collaborations with the HyMARC team.

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INTRODUCTION

The Hydrogen Storage program supports research and development of technologies to lower the cost of near-term physical storage options and longer-term material-based hydrogen storage approaches. The program conducts R&D of low-pressure, materials-based technologies and innovative approaches to increase storage potential and broaden the range of commercial applications for hydrogen. These advanced materials activities focus on development of core capabilities designed to enable the development of novel materials with the potential to store hydrogen near room temperature, at low-to-moderate pressures, and at energy densities greater than either liquid or compressed hydrogen on a systems basis. Key activities include improving the energetics, temperature, and rates of hydrogen release. Advanced concepts include high-capacity metal hydrides, chemical hydrogen storage materials, and hydrogen sorbent materials, as well as novel material synthesis processes. The overarching goal of the Fuel Cell Technologies Office Hydrogen Storage program is to develop and demonstrate viable hydrogen storage technologies for transportation, stationary, portable power, and specialty vehicle applications (e.g., material handling equipment, airport ground support equipment), with a key goal of enabling >300-mile driving range across all light-duty vehicle platforms, without reducing vehicle performance or passenger cargo space.

APPROACH

This national laboratory collaboration between NREL, PNNL and LBNL, and NIST brought together internationally recognized leaders in hydrogen storage materials characterization and development. This collaboration is predicated on a synergistic approach to further validate hydrogen storage concepts and develop the key core-capabilities necessary for accurate evaluation of hydrogen storage materials capacity, kinetics, and sorption and desorption physio-chemical processes. The overall approach involves collaborative experimental and modeling efforts. We are validating concepts and utilizing core capabilities to rapidly define, model, synthesize, and characterize the appropriate materials necessary for achieving the 2020 Hydrogen Storage goals set forth by DOE. The approach is multifaceted to mitigate risk and ensure success as we bridge the gap between physisorption and chemisorption to provide the basis for a new generation of hydrogen storage materials technologies.
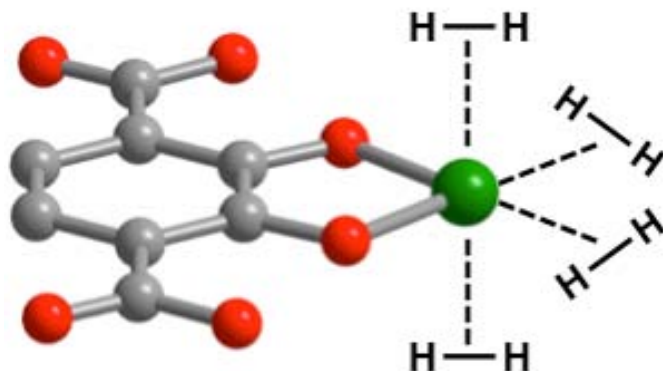
Our work in FY 2016 included efforts to develop state-of-the-art characterization techniques for hydrogen storage in thermal conductivity, infrared spectroscopy and NMR spectroscopy. Through a theoretical and experimental interaction, we focused on the validation of recently provocative concepts in hydrogen storage including the possibility of multiple hydrogen molecules being adsorbed on

an unsaturated metal center within a sorbent. Is it possible to enhance the kinetics of hydride formation with additives, and how can one alter or increase the hydrogen binding energies for physisorption in non-crystalline and crystalline sorbents?

RESULTS

Concept Validation

The goal of FY 2016 was our primary go/no-go decision: determine if more than one hydrogen molecule can adsorb to an unsaturated metal center in a sorbent material (Figure 1). The most notable result was the discovery of a material that can bind two hydrogen molecules to a single metal center. This material, Mn_2(dsbdc) ($dsbdc^{4-}$ = 2,5-disulfido-benzene-1,4-dicarboxylate), features a similar structure to the well known Mn_2(dobdc) analog, yet exhibits structural differences that result in the ability of this material to bind two H_2 molecules to a single metal center. In particular, the ligand contains sulfido groups rather than oxido groups, leading to a different geometry around the metal centers. Thus, rather
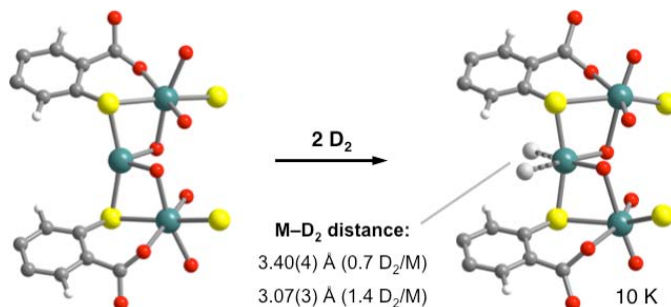
than having five-coordinate metal centers with the sixth coordination site occupied by a solvent molecule, Mn_2(dsbdc) exhibits alternating four- and six-coordinate Mn^{2+} centers down the *c* axis. Two solvent molecules can be removed from the four-coordinate Mn^{2+} center, resulting in two open metal centers. Gratifyingly, D_2-dosed powder neutron diffraction studies determined that two D_2 molecules bind to this single Mn^{2+} center, as expected (Figure 2). This is the first example of two H_2 (D_2) molecules binding to a single metal center in a metal organic framework (MOF).

In our attempts to control the desorption temperature of the hydrogen from sorbents we investigated a series of oxo-carbon species with different metal centers. Since the modeling had predicted the trends for hydrogen binding energies, we investigated specifically a series of metal croconate ($C_5O_5^{2-}$) and metal-oxalate ($C_2O_4^{2-}$) species (Figure 3).

Another notable accomplishment this year has been the development of a reaction scheme to predict key intermediates in the reversible decomposition of $Mg(BH_4)_2$. The reaction scheme (Scheme 1) utilizes (i) a modification of the "BH condensation pathway," [1] to provide a rational reaction pathway for the clustering of the borane molecules,

FIGURE 1. Illustration of an unsaturated metal center with multiple hydrogen molecules attached to the metal center

M–D_2 distance:
3.40(4) Å (0.7 D_2/M)
3.07(3) Å (1.4 D_2/M)

10 K

FIGURE 2. First demonstration of two H_2 molecules binding to a metal center in a metal organic framework. Mn_2(dsbdc)
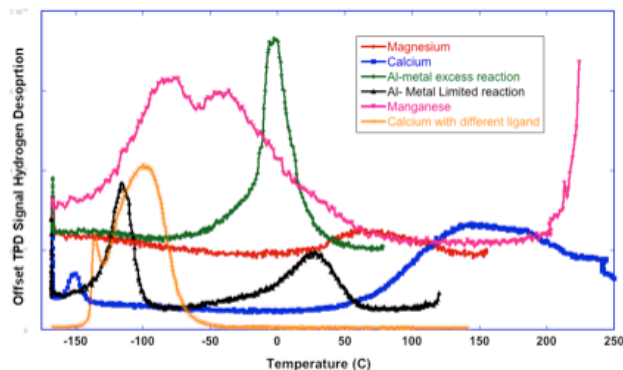

Metal/Ligand	Desorption Temperature (K)	Gravimetric capacity (1 bar) %w/w approximate
Be/mixed oxalate	150 K	<0.2%
Al/mixed oxalate	125 – 175 K (small pk 273K)	0.1 – 0.3%
Ca/mixed oxalate	150 – 225K	0.4 – 0.8%
Mg/croconate	340K	<0.1%
Ca/Croconate	350 – 473 K	<0.1%
Al/Croconate (a)	265 – 290 K	0.5 – 0.8%
Al/croconate (b)	140 – 170 K, 273 – 320K	0.1 – 0.3%
Mn/Croconate	200 K and 225 K (2 peaks)	0.2 – 0.4%

FIGURE 3. Left: Temperature programmed desorption (TPD) experiments for a series of M-croconate and metal-oxalate species. Samples were exposed to 1 bar hydrogen at 298 K for 10 min, quenched with liquid nitrogen, headspace evacuated to 10^{-8} torr and then heated at 10 K/min. Key observation: through experimental conditions (e.g., metal type, reagent concentrations), the hydrogen desorption temperatures were significantly affected. Right: table summarizing TPD results.

that can be formed under the reaction conditions (i.e., hydrides and H_2) and (ii) "Wades Rules" which provide a set of rules to define the connectivity of closo, nido, archno, and hypo borane clusters. Scheme 1 below shows an example of the reversible pathways linking BH_4^- to the closo-$B_{10}H_{10}$ dianion. This scheme provides a critical starting point that uses a rational explanation to predict key intermediates. This approach contrasts published literature where a great number of borane clusters have been proposed with little rationale of why they would form under the set of reaction conditions.

Another part of our effort was to model a series of metal-catecholate-based materials for the possible binding of multiple hydrogen molecules. The goal is part of our inverse design effort to determine the best unsaturated metal center for enhanced binding energies. A summary of the results is shown in Figure 4. From this effort, we are now pursing a
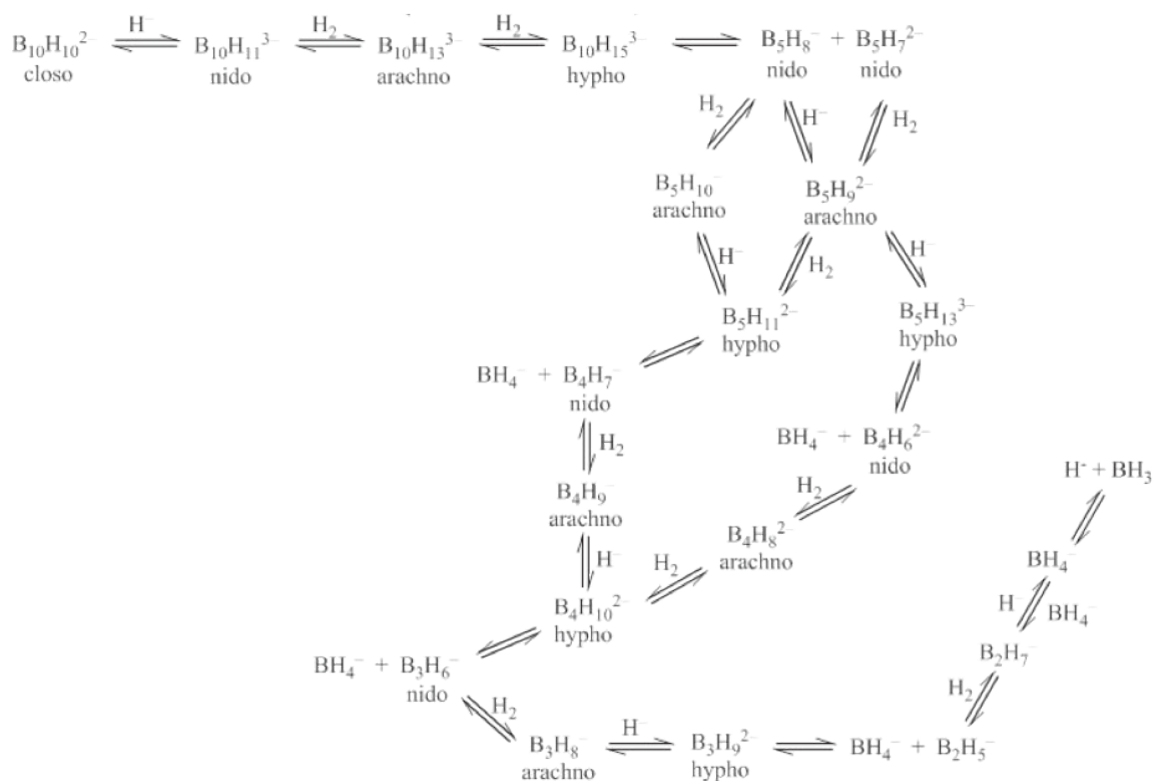
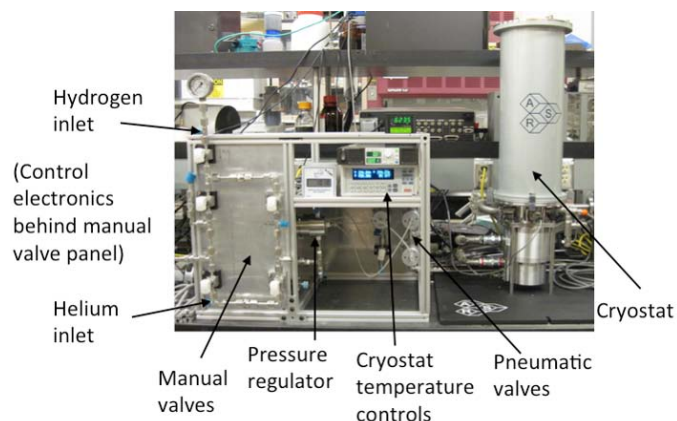**SCHEME 1.** Proposed reversible reaction pathway for BH_4^- to $B_{10}H_{10}$
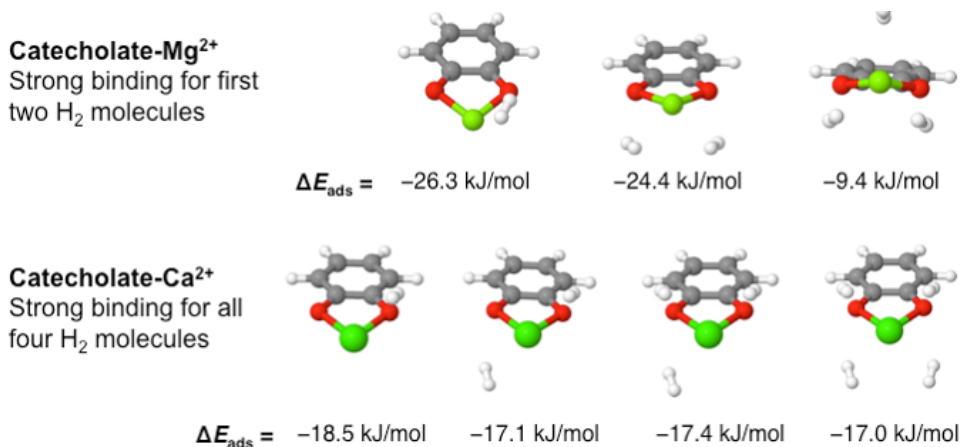
FIGURE 4. Calculated adsorption and binding energies for multiple hydrogen molecules bound to an unsaturated catecholate-M^{2+} species.

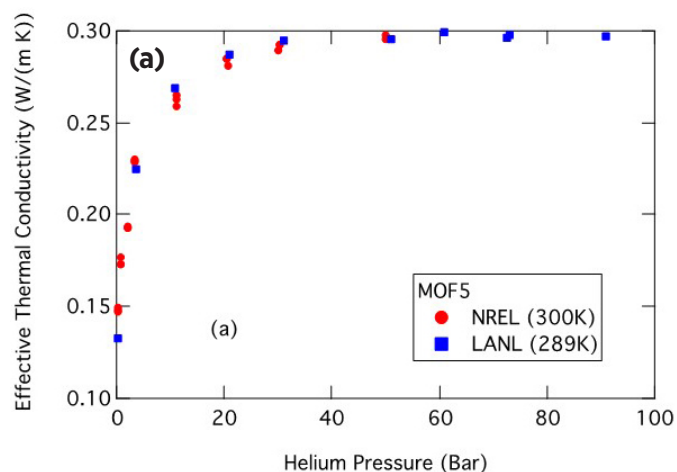series of calcium-based framework and oxocarbon materials to test the model.

Characterization Techniques and Validation of Performance

In FY 2016 we designed and constructed a new advanced thermal conductivity apparatus capable of measuring the thermal conductivity of hydrogen storage materials under expected operating conditions. We have developed the instrument to enable measurements at temperatures from 50 to 380 K with up to 100 bar overpressure of gas. It is amenable to the evaluation of both pucks and powders. A picture of the apparatus is shown in Figure 5, and the validation of performance in Figure 6.

Another key objective in FY 2016 was to compare and contrast the results of a round-robin experiment to determine the gravimetric and volumetric capacities of two standard materials. A detailed protocol on how to degas the materials and prep them for measurement was included. A run sheet was included so all experimental conditions could be recorded and sent with the results. The round robin was initiated in December 2015, and while all the results are still not in, a sampling of the results is shown in Figure 7. We are working with all the participants and going over calculations and protocols, especially for those whose results seemed to have some systematic error. This hydrogen-storage characterization study assesses the accuracy of excess and total volumetric capacities measurements within the hydrogen storage community. Knowledge of the measurement accuracy enables meaningful comparison of the sorption capacities.

In FY 2016 we also have developed the engineering design for a new advanced diffuse reflectance infrared Fourier transform spectroscopy spectrometer that will be able to measure from 20–373 K with overpressures up to 100 bar. This instrument is expected to come online in FY 2017. Because of non-disclosure agreement limitations, the design and manufacturer cannot be disclosed at this time.

Finally in FY 2016 we developed a new utilization of advanced NMR spectroscopy techniques under a series of hydrogen overpressures at different temperatures and for different nuclei. One of most significant results was to be the first to measure the static solid state ^{1}H NMR spectra of H_2 physisorbed to Mg_2(*m*-dobdc) MOF. We are investigating approaches to extract T_1 relaxation data to gain insight into the binding energy of H_2 to a metal center in high surface area materials. In the next year we will develop dynamics models to fit experimental NMR data. NIST neutron (quasielastic neutron scattering and inelastic neutron scattering) and LBNL Fourier transform infrared will complement the NMR experiments. We have also calculated the Pake pattern of what should be observed for the ^{1}H

FIGURE 5. The assembled thermal conductivity apparatus for hydrogen storage materials
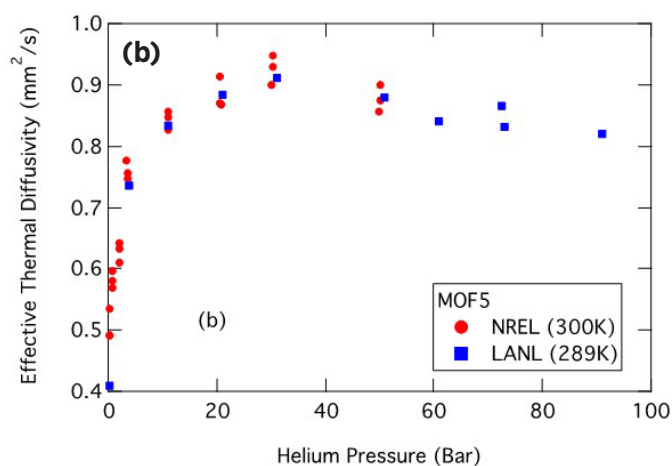
FIGURE 6. Measured thermal conductivity (a) and thermal diffusivity (b) of a MOF-5 sample in helium as a function of helium pressure. The performance was validated via a comparison to the fixed-temperature apparatus at LANL (Troy Semelsberger).
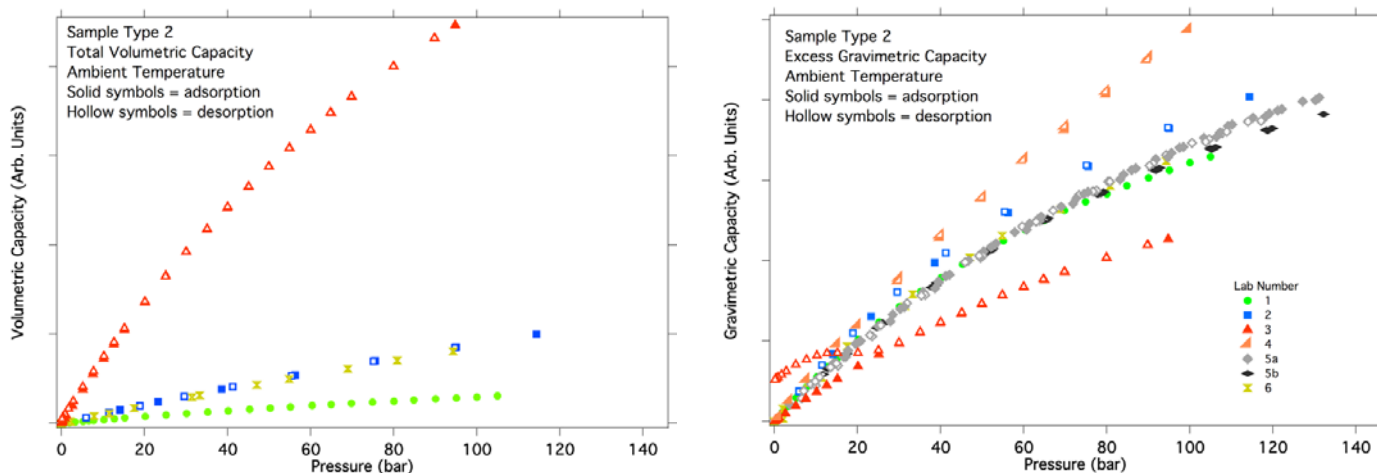
FIGURE 7. Sampling of results from the round robin. These results only represent those done at room temperature for Sample 2. We are also compiling 77 K data for both samples as well. Left: Range of the *total* volumetric capacities reported at room temperature, Right: Range of *excess* gravimetric capacity for Sample 2 at room temperature.

NMR spectra for two tightly bound hydrogen molecules per metal site.

CONCLUSIONS AND FUTURE DIRECTIONS

Our collaboration has provided us with the opportunity to validate several key aspects of hydrogen storage materials that were first reported in FY 2016. These include binding two hydrogen molecules to a metal center in a framework material (which was the Performance Evaluation and Measurement Plan milestone and go/no-go within FY 2016), controlling the binding energy by changing metal centers in model oxo-carbon species, increasing the binding energy in carbon sorbents by the introduction of catecholates and metal centers, improving the kinetics and elucidating the possible favorable pathways for the reversible hydrogenation of magnesium borohydride, validating several models or predictions of materials, developing advanced techniques that have already had a significant impact in the community, and establishing the effect of systematic error on the reported capacities of standard carbon materials. Taken together these results have established a multitude of possible solutions for advanced hydrogen storage materials, both sorbents and hydrides. Our future work will now work to continue our development of several new characterization tools in FY 2017 that will be essential to the DOE Fuel Cell Technologies Office hydrogen storage programs. We will also focus our efforts to continue to look at inverse designed materials as we strive to increase the capacity of the new genre of hydrogen sorbents and improve the reversibility kinetics of possible hydrides. Furthermore, we will also look at the validation of concepts associated with the claims that boron- and nitrogen-doped sorbents are possible materials for increased binding energies of physisorption; address the questions: (1) will the insertion of calcium into framework materials increase binding energy as predicted, and (2) is it possible to have the attachment of >2 hydrogen molecules; and finally, evaluate the application to heterolytic cleavage of hydrogen as a possible mechanism to reach the 2020 targets.

SPECIAL RECOGNITIONS & AWARDS/PATENTS ISSUED

1. Jeff Long and Craig Brown received the DOE Fuel Cell Technologies Office Outstanding Achievement award at the June 2016 AMR meeting

FY 2016 PUBLICATIONS

1. "Hydrogen Storage in the Expanded Pore Metal-Organic Frameworks M_2(dobpdc) (M = Mg, Mn, Fe, Co, Ni, Zn)," Gygi, D.; Bloch, E.D.; Mason, J.A.; Hudson, M.R.; Gonzalez, M.I.; Siegelman, R.L.; Darwish, T.A.; Queen, W.L.; Brown, C.M.; Long, J.R. *Chem. Mater.* **2016**, *28*, 1128–1138.

2. "Adsorption of Two Gas Molecules at a Single Metal Site in a Metal-Organic Framework," Runčevski, T.; Kapelewski, M.T.; Torres-Gavosto, R.M.; Tarver, J.D.; Brown, C.M.; Long, J.R., *Chem. Commun.* **2016**, *52*, 8251–8254.

3. "Hydrogen Storage and Selective, Reversible O_2 Adsorption in a Metal-Organic Framework with Open Chromium(II) Sites," Bloch, E.D.; Queen, W.L.; Hudson, M.R.; Mason, J.A.; Xiao, D.J.; Murray, L.J.; Flacau, R.; Brown, C.M.; Long, J.R., Angew.Chem. Int.Ed. 2016, 55,8605 –8609.

4. "Olsalazine-Based Metal-Organic Frameworks as Biocompatible Platforms for H_2 Adsorption and Drug Delivery," Levine, D.J.; Runčevski, T.; Kapelewski, M.T.; Keitz, B.K.; Oktawiec, J.; Reed, D.A.; Mason, J.A.; Jiang, H.Z.H.; Colwell, K.A.; Legendre, C.; FitzGerald, S.A.; Long, J.R., *J. Am. Chem. Soc.,* 2016, 138 (32), pp 10143–10150

5. "An International Multi-Laboratory Investigation of Carbon-Based Hydrogen Sorbent Materials," Hurst, K.E.; Parilla, P.A.; O'Neill, K.J.; Gennett T. *Appl. Phys. A* **2016**, *122*, 42.

6. "Recommended Volumetric Capacity Definitions and Protocols for Accurate, Standardized and Unambiguous Metrics of Hydrogen Storage Materials," Parilla, P.A.; Gross, K.; Hurst, K.E.; Gennett, T. *Appl. Phys. A* **2016**, *122*, 201.

7. "Outlook and Challenges from Hydrogen Storage in Nanoporous Materials," Broom, D.P.; Webb, C.J.; Hurst, K.E.; Parilla, P.A.; Gennett, T.; Brown, C.M.; Zacharia, R.; Tylianakis, E.; Klontzas, E.; Froudakis, G.E.; Steriotis, Th.A.; Trikalitis, P.N.; Anton, D.L.; Hardy, B.; Tamburello, D.; Corgnale, C.; van Hassel, B.A.; Cossement, D.; Chahine, R.; Hirscher, M. *Appl. Phys. A* **2016**, *122*, 151.

8. "Dynamics of Pyramidal SiH_3 Ions in $ASiH_3$ (A = K and Rb) Investigated with Quasielastic Neutron Scattering," Österberg, C.; Fahlquist, H.; Häussermann, U.; Brown, C.M.; Udovic, T.J.; Karlsson, M. *J. Phys. Chem. C* **2016**, *120*, 6369−6376.

9. "Complex and Liquid Hydrides for Energy Storage," Callini, E.; Özlem, Z.; Atakli, K.; Hauback, B.C.; Orimo, S.; Jensen, C.; Dornheim, M.; Grant, D.; Cho, Y.W.; Chen, P.; Hjörvarsson, B.; deJongh, P.; Weidenthaler, C.; Baricco, M.; Paskevicius, M.; Jensen, T.R.; Bowden, M.E.; Autrey, T.S.; Züttel, A. *Appl. Phys. A* **2016**, *122*, 353.

10. "A Chemistry Perspective on Reversible Reaction Pathways Enabling Hydrogen Storage in Magnesium Borohydride," Edvenson, G.; Chong, M.; Autrey, T.; Jensen, C. Invited Feature Article in *Chem. Commun.*

11. "HyMARC-H_2 Core : Nanointerface-driven Reversible Hydrogen Storage in the Nanoconfined Li-N-H System," Wood, B.C.; Stavila, V.; Poonyayant, N.; Heo, T.W.; Ray, K.G.; Klebanoff, L.E.; Udovic, T.J.; Lee, J.R.I.; Angboonpong, N.; Pakawatpanurut, P, *Nature Mater.* response to reviewers submitted.

12. "Structure-Dependent Vibrational Dynamics in $Mg(BH_4)_2$ Polymorphs Probed with Neutron Vibrational Spectroscopy and First-Principles Calculations," Dimitrievska, M.; White, J.L.; Zhou, W.; Stavila, V.: Klebanoff, L.E.; Udovic, T.J. *Phys. Chem. Chem. Phys*, 2016,18, 25546-25552.

13. "Structural and Dynamical Trends in Alkali-Metal Silanides Characterized by Neutron Scattering Methods," Tang, W.S.; Dimitrievska, M.; Chotard, J.-N.; Zhou, W.; Janot, R.; Skripov, A.V.; Udovic, T.J.; *J. Phys. Chem. C, DOI: 10.1021/acs.jpcc.6b06591.*

14. "Vibrational Properties of β-$KSiH_3$ and β-$RbSiH_3$: A Combined Raman and INS Study," Mink, J.; Lin, Y-C; Karlsson, M.; Österberg, C.; Udovic, T.J. ; Fahlquist, H.; Häussermann, U.; *J. Raman Spectroscopy,* DOI 10.1002/jrs.5013.

FY 2016 PRESENTATIONS

1. *NREL Core Capabilities, a Review*, T. Gennett joint HyMARC meeting, 11/4/2015.

2. *Advances in Hydrogen Sorption: Sorbent and Hybrid Sorbent-Hydride, Characterization, and Validation*, P. Parilla, K. Hurst, M. Olsen, J. Blackburn, A. Dameron and T. Gennett at Pacific Chem. Honolulu, HI. 12/18/15

3. *Hydrogen Sorption Capacity Protocols*, K. Hurst, P. Parilla, K. Gross, and T. Gennett at the International Hydrogen and Energy Symposium Zao, Japan 2/21-16/2016.

4. *The Effect of Coordinated Metal Centers on Binding Energy in Non-Crystalline Materials*, K. Hurst, P. Parilla, M. Olsen, J. Blackburn, A. Dameron and T. Gennett at the IEA-HIA meeting, Sendai, Japan 2/27/2016.

5. *Research and Development of Advanced Hydrogen Storage Core Characterization Techniques and Materials*, Tom Gennett, Jeff Long, Craig Brown, Mark Bowden, Abhi Karkamkar, Tom Autrey at the International Hydrogen and Energy Symposium Zao, Japan 2/16-21, 2016.

6. *Hydrogen Storage Capacity Protocols K*.E. Hurst, P.A. Parilla, K. Gross, T. Gennett International Hydrogen and Energy Symposium Zao, Japan February 16–21, 2016.

7. *Variable-Pressure, Variable-Temperature Measurement of the Thermal Properties of Hydrogen Storage Materials,* Michele Olsen, Philip Parilla, Katherine Hurst, Thomas Gennett at MRS Spring Meeting, 4/1/2016.

8. *Hydrogen Storage Characterization Optimization and Research Effort, an Overview.* T. Gennett H_2ST^2 Tech Team review, 4/20/16.

9. *Hydrogen Storage Characterization and Research Optimization Effort: LBNL,* Jeff Long, Martin Head-Gordon H_2ST^2 Tech Team review, 4/20/16.

10. *Hydrogen Storage Characterization and Research Optimization Effort: PNNL,* Tom Autrey, Mark Bowden H_2ST^2 Tech Team review, 4/20/16.

11. *Hydrogen Storage Characterization and Validation Efforts*, T. Gennett, P. Parilla, J. Blackburn, A. Dameron, M. Olsen, K. Hurst, J. Tynan, S. Robbins, S. Ferrere, A. Dameron. H_2ST^2 Tech Team Review 4/20/16.

12. *Hydrogen Storage Characterization and Research Optimization Effort: NIST*, Craig Brown, Terry Udovic H_2ST^2 Tech Team Review 4/20/16.

13. *H_2 Storage Characterization and Optimization Research Effort,* Rory Andrykowski, Jeff Blackburn, Arrelaine Dameron, Mira Dimitrievska (NIST), Suzanne Ferrere, Katie Hurst, Michele Olsen, Phil Parilla, Steve Robbins, Jacob Tarver (NIST), Jerry Tynan, Tom Gennett (PI) DOE Hydrogen and Fuel Cells Program Annual Merit Review, 6/8/2016.

14. *Hydrogen Sorbent Measurement Qualification and Characterization,* Phil Parilla, Katherine Hurst, Michele Olsen, Steve Robbins, Jerry Tynan, Tom Gennett. DOE Hydrogen and Fuel Cells Program Annual Merit Review, 6/8/2016.

15. *H_2 Storage Characterization and Optimization Research Effort,* Craig Brown (NIST), Terrence Udovic (NIST), Jacob Tarver (NREL), Mirjana Dimitrievska (NREL) and Thomas Gennett (NREL). DOE Hydrogen and Fuel Cells Program Annual Merit Review, 6/8/2016.

16. *H_2 Storage Characterization and Optimization Research Effort,* Jeffrey Long, Martin Head-Gordon, DOE Hydrogen and Fuel Cells Program Annual Merit Review, 6/8/2016.

17. *H₂ Storage Characterization and Optimization Research Effort,* Tom Autrey, Mark Bowden, Abhi Karkamkar, Bojana Ginovska, Herman Cho, Marina Chong, Adrian Houghton, Gary Edvenson, DOE Hydrogen and Fuel Cells Program Annual Merit Review, 6/8/2016.

18. *Oxocarbon-Metal Microporous Channel Materials for Gas Sorption*, Thomas Gennett, Jacob Tarver, Katherine Hurst, Jeffrey R. Long, Tom Autrey, Mark Bowden and Craig Brown, 5th International Conference on Metal-Organic Frameworks and Open Framework Compounds 9/13/2016.

19. *PNNL Core NMR Capabilities and Application to Hydrogen Storage Materials Characteization,* T. Autrey, M. Bowden joint HyMARC meeting, 11/4/2015.

20. *Infrared Spectroscopy Applied to Hydrogen Storage in Metal-Organic Frameworks and Porous Polymers,* Matthew Kapelewski, Henry Jiang, Tomce Runcevski, Gokhan Barin, Mercedes Taylor, Ehud Tsivion, Martin Head-Gordon, Jeffrey Long joint HyMARC meeting, 11/4/2015.

21. *Structural and Dynamical Trends in Alkali-Metal Silanides Characterized by Neutron Scattering Methods*, Pacifichem 2015, Honolulu, HI, T.J. Udovic, December 18, 2015.

22. *NIST Center for Neutron Research an Overview of Capabilities*, C. Brown, T. Udovic joint HyMARC meeting, 11/4/2015.

23. *H₂ Storage on Open Metal Coordination Sites–Best Performance in Ni₂(m-dobdc) and Two H₂ Molecules on One Metal in Mn₂(dsbdc)***,** Matthew T. Kapelewski, Tomče Runčevski, Henry Z. Jiang, Katherine E. Hurst, Thomas Gennett, Stephen A. FitzGerald, Craig M. Brown, and Jeffrey R. Long. 5th International Conference on Metal-Organic Frameworks & Open Framework Compounds (MOF 2016). Long Beach, CA, 9/15/2016.

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