University of Missouri

New Pathways and Metrics for Enhanced, Reversible Hydrogen Storage in Boron-Doped Carbon Nanospaces

Progress Report 5 (Final Report)

DOE Award:	DE-FG02-07ER46411
Recipient Institution:	University of Missouri
Project Title:	Phase I: *Networks of Boron-Doped Carbon Nanopores for Low-Pressure Reversible Hydrogen Storage.* Phase II: *New Pathways and Metrics for Enhanced, Reversible Hydrogen Storage in Boron-Doped Carbon Nanospaces*
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I - Project Scope

This project, since its start in 2007—entitled "Networks of boron-doped carbon nanopores for low-pressure reversible hydrogen storage" (2007-10) and "New pathways and metrics for enhanced, reversible hydrogen storage in boron-doped carbon nanospaces" (2010-13)—is in support of the DOE's National Hydrogen Storage Project, as part of the DOE Hydrogen and Fuel Cells Program's comprehensive efforts to enable the widespread commercialization of hydrogen and fuel cell technologies in diverse sectors of the economy. Hydrogen storage is widely recognized as a critical enabling technology for the successful commercialization and market acceptance of hydrogen powered vehicles. Storing sufficient hydrogen on board a wide range of vehicle platforms, at energy densities comparable to gasoline, without compromising passenger or cargo space, remains an outstanding technical challenge. Of the main three thrust areas in 2007—metal hydrides, chemical hydrogen storage, and sorption-based hydrogen storage—sorption-based storage, i.e., storage of molecular hydrogen by adsorption on high-surface-area materials (carbons, metal-organic frameworks, and other porous organic networks), has emerged as the most promising path toward achieving the 2017 DOE storage targets of 0.055 kg H_2/kg system ("5.5 wt%") and 0.040 kg H_2/liter system.

The objective of the project is to develop high-surface-area carbon materials that are boron-doped by incorporation of boron into the carbon lattice *at the outset*, i.e., during the synthesis of the material. The rationale for boron-doping is the prediction that boron atoms in carbon will raise the binding energy of hydrogen from 4-5 kJ/mol on the undoped surface to 10-14 kJ/mol on a doped surface, and accordingly the hydrogen storage capacity of the material. The mechanism for the increase in binding energy is electron donation from H_2 to electron-deficient B atoms, in the form of sp^2 boron-carbon bonds. Our team is proud to have demonstrated the predicted increase in binding energy experimentally, currently at ~10 kJ/mol.

The synthetic route for incorporation of boron at the outset is to create appropriately designed copolymers, with a boron-free and a boron-carrying monomer, followed by pyrolysis of the polymer, yielding a boron-substituted carbon scaffold in which boron atoms are bonded to carbon atoms by synthesis. This is in contrast to a second route (funded by DE-FG36-08GO18142) in which first high-surface area carbon is created and doped by surface vapor deposition of boron, with incorporation of the boron into the lattice the *final step* of the fabrication. The challenge in the first route is to create high surface areas without compromising sp^2 boron-carbon bonds. The challenge in the second route is to create sp^2 boron-carbon bonds without compromising high surface areas.

a) *Networks of Boron-Doped Carbon Nanopores for Low-Pressure Reversible Hydrogen Storage*. The first DOE award provided a total of $880,000 over the period 08/15/2007 through 08/14/2010. The research funded by this grant has resulted in the development of nanoporous carbon with record-breaking H_2 storage: gravimetric excess adsorption of 0.073 ± 0.003 kg H_2/kg C (7.3 wt%), gravimetric storage capacity of 0.107 ± 0.005 kg H_2/kg carbon (11 wt%), and volumetric storage capacity of 0.040 ± 0.003 kg H_2/liter carbon, at T = 80 K and p = 50 bar. In addition, significant developments were made on the: production of monodisperse nanoporous structures; on the chemical modification of carbons with boron; on the methodology to characterize the nanometer-scale pore structure of the materials (SAXS, adsorption isotherms aided by theoretical and computational results, inelastic neutron scattering); on the development of reliable computational methods to guide the creation of new nanoporous structures; and on the determination from first principles of the interaction potential between hydrogen molecules and boron containing carbon substrates.

The research project consisted of an integrated synthesis, characterization, and computational effort to develop novel materials—monolithic boron-doped carbon made from polymeric precursors, crisscrossed by networks of nanopores—expected to have superior hydrogen storage capacities not available in other materials. The aim was to develop a fundamental understanding of the mechanisms by which boron, through its electron-deficient electronic structure and long-range effect on distant carbon atoms, combined with appropriate pore geometries, creates deep potential wells which can hold films of physisorbed molecular hydrogen at densities much higher than undoped carbon. Such high-density films and their understanding at the molecular, statistical mechanical, and macroscopic thermodynamic level are critical for the rational design of high-performance materials with controlled reversible storage characteristics at low pressure and room temperature. Characterization of the carbons was undertaken in a multi-pronged approach. Carbons were systematically studied by sub-critical N_2 adsorption (determination of BET surface areas, pore-size distribution), transmission electron microscopy and small-angle x-ray scattering (SAXS). Typically, activated carbons show a broad distribution of pore sizes in the sub-nm to tens of nm range. The existence of this broad range of pore sizes is consistent with the analysis of pore size distribution from H_2 adsorption isotherms which show that a bimodal distribution of pore sizes results in a two-binding energy (BE) model for adsorption (narrow pores: BE = ~9 kJ/mol, wide pores: BE = ~5 kJ/mol). For most synthetic carbons, the pore size distribution is predominantly monodisperse, with a high fraction of sub-nm pores, consistent with the pore-drilling mechanism of PVDC (-[(CH_2)-(CCl_2)]- → 2C + 2HCl). SAXS analysis of PVDC samples is consistent with this view, as are the H_2 adsorption isotherms.

The nanoporous carbon storage capacities found so far have lead us to understand that a pore-space architecture that simultaneously maximizes gravimetric and volumetric storage capacities will likely consist of graphitic sheets that hold 2-3 layers of H_2 between adjacent sheets. A variety of interaction potentials were considered computationally and down-selected by comparison with experimental adsorption data. At cryogenic temperatures Feynman-Hibbs quantum corrections are important both for H_2-substrate and for H_2-H_2 interactions, and we also found that some multi-layer adsorption was likely important. Two theoretical models were analyzed for the Langmuir adsorption of H_2 onto nanoporous carbon. We either considered that adsorption was mobile (more precisely onto a continuous set of adsorption sites) or localized (onto a discrete set of adsorption sites). Comparison of adsorbed densities of H_2 in nanoporous carbon to experimental isotherms leads us to conclude that adsorption is mostly onto localized sites at 77 K and mostly mobile at 298 K. Our results highlight the fact that hydrogen itself may be used as a probe into the structure and function of nanoporous materials.

b) *New Pathways and Metrics for Enhanced, Reversible Hydrogen Storage in Boron-Doped Carbon Nanospaces*. The second DOE award, provided a total of $960,000 over the period 08/15/2010 through 08/14/2013. The research funded by the award focused on the synthesis of new materials and their characterization in terms of structure and function as hydrogen storage materials (including binding energies of adsorbed hydrogen films), the design and construction of a 20-K hydrogen sorption analyzer, designed for high-precision hydrogen isotherms at the normal boiling point of hydrogen; the discovery and analysis that some of these materials have expandable pore spaces (which is of great interest for dynamically adjustable storage capacities); the discovery that adsorbed hydrogen films behave like liquids, with well-defined, sub-nanometer film thicknesses and film densities higher than in bulk liquid hydrogen, under conditions at which no liquid should exist according to macroscopic thermodynamics, giving rise to new, unanticipated metrics for high-capacity hydrogen storage; on computational work that predicts other pathways to high-capacity hydrogen storage ("open carbon frameworks"); and on insight into the dynamics of adsorbed hydrogen films by inelastic neutron scattering (collision-induced recoil of hydrogen molecules on locally planar surfaces).

The project has resulted in one patent, 116 publications and presentations, including 21 papers published in journals such as *J. Am. Chem. Soc.*, *Phys. Rev.*, *Carbon*, etc.; 4 Ph.D. dissertations completed (3 additional ones will be completed before the end of 2014); and 1 M.S. thesis completed. The project also resulted in 26 invited talks at national and international conferences, seminars and colloquia; and 65 contributed presentations (oral, poster) in conferences (mostly by our graduate and undergraduate students). The project has supported three sabbatical visits by Prof. Bogdan Kuchta (Univ. Marseille, France, 0.5 FTE) and Prof. Lucyna Firlej (Univ. Montpellier 2, France, 0.5 FTE), 1 Assistant Research Professor (1.0 FTE), 1 postdoc (0.5 FTE), 8 graduate students (0.5 FTE on average), and 10 undergraduate students. The project also provided essential stimulus, although no financial support by directive of DOE/BES, to hold the conference "Adsorption at the Nanoscale," University of Missouri, September 22-24, 2011, with over 90 participants from nine countries. The conference was widely regarded as a great success.

II – Accomplishments

Our group has focused on the development of materials derived from synthetic precursors in order to optimize, measure, and control pore geometries at the sub-nm scale; and to enhance the adsorption of H_2 by increasing the depth of the adsorption potential by chemical functionalization of the surface. We have spearheaded this effort to improve these materials and have reported:

(i) Record-breaking H_2 storage in very high-surface area activated carbons (Fig. 1); [References 13, 15, 16, 21, 22, 23, 24]

(ii) In graphene, our *ab initio* calculations indicate that doping with boron can rise the binding energy of a single graphene plane significantly (see Fig. 2), resulting in BE >12 kJ/mol in 1.2 nm wide slit-shaped pores at 10% B/C. Grand Canonical Monte Carlo simulations of H_2 adsorption in such systems result in dramatically enhanced adsorption of H_2, with room temperature storage capacities of ~6 wt% achievable at moderate pressures, thus showing the potential that boron-doped carbon may be the first system capable of achieving the 2010 DOE goals (excluding tank enclosure, pumps, etc.). [References 11, 12, 14, 19, 20, 23, 24]

(iii) Grand canonical Monte Carlo simulations that successfully reproduce the experimental adsorption isotherms of H_2 in heterogeneous pore structures, and that demonstrated enhanced H_2 adsorption in B-doped carbon; See Fig. 2. [References 7, 8, 9, 10, 17, 19, 20, 23, 24]

(iv) Demonstrated experimentally the existence of B-C bonds in B-doped carbon; [Reference 2, 16, 23, 24]

(v) Demonstrated experimentally that in B-doped carbons the isosteric heat of adsorption nearly doubles from 5-7 kJ/mol to 9-12 kJ/mol, in agreement with our theoretical predictions; [References 15, 16, 23, 24]

(vi) Demonstrated that activated carbon from synthetic precursors have a nearly monodisperse network of narrow pores (Fig. 3, right); [References 15, 16, 17, 23, 24]

(vii) Developed pore characterization methods based on small-angle X-ray scattering (SAXS); [Reference 18, 23, 24]

(viii) Developed the theoretical background to utilize incoherent inelastic neutron scattering (IINS) off adsorbed H_2 to characterize the interaction potentials as seen by molecular H_2 in sub-nm pores. See Fig. 4. [References 6, 17, 23, 24]

(ix) IINS is capable of probing both energy levels and quantum states of adsorbed H_2 directly. We conducted experiments at ORNL over an unprecedented broad range of energy and momentum transfer, observing as expected the 1st rotational transition ($E_1 - E_0$) at 14.7 meV and a roto-vibrational peak at 29.5 meV for a variety of carbon samples: multi-walled carbon nanotubes, activated carbons MSC-30 and 3K-600C, and HS;0B-20, see Fig. 4). Similarities of spectra for samples with very different PSDs (not shown) suggest (except HS;0B) very few sub-nm pores in activated carbons, most pores with similar binding energies. We developed a novel theoretical methodology that permitted the classification of the H_2 excitations into localized and mobile states, allowing for a measure of the planarity of the adsorption surface on the > 1 nm scale. [References 1, 17, 23]

(x) Observed anomalous adsorption of H_2 in synthetic carbon: significantly higher excess adsorptions normalized per Brunauer-Emmett-Teller (BET) surface area at both cryogenic and room temperature (Fig. 1), which indicates higher binding energies (consistent with a narrower pores). [References 15, 16, 23, 24]

(xi) We have successfully designed and constructed a sub- and super-critical H_2 Sievert sorption instrument to be used for sub-critical and super-critical H2 adsorption (temperature range: 4-300+ K). See Fig. 5. The 20-K hydrogen sorption analyzer is a dosing-type, Sievert apparatus designed to measure isotherms from 0.01-200 bar with various gases including hydrogen, helium, methane, nitrogen and carbon dioxide. Either a closed-cycle helium refrigerator (7 K to 298 K) or a tube furnace (298 K to 600 K) controls the temperature. The closed-cycle refrigerator has a temperature stability of ±5 mK. The sample cell can hold sample sizes from 0.5 g up to approximately 3g. It has two pressure transducers, one low pressure (0.01-2 bar) and one high pressure (1.7-340 bar). This configuration allows the instrument to measure isotherms accurately for the entire pressure range of 0.01 to 200 bar. All connections are VCR metal gasket fittings, which allows the system to be easily modified and leak free. The valves are pneumatically controlled. Pneumatic valves have the benefit that they do not heat up during use, as compared to electronic valves, which can warm up significantly. This is important for the sorption measurements, as the dosing volume needs to remain at a constant temperature. The apparatus is controlled by a LabVIEW program that was written in-house. This program controls the valves and closed-cycle refrigerator temperature and reads in the pressure and temperature data. It then calculates the gas uptakes from the data and produces a report of the sample isotherm. The high pressure and low temperatures that this instrument can achieve allow for two different and unique experiments. First, this allows for hydrogen isotherms at subcritical temperatures (T < 33.0 K). The second experiment that this instrument makes possible is high pressure measurements at supercritical temperatures but at colder than typical temperatures (33.0 K < T < 77 K). At these high pressures (up to 200 bar) and cold temperatures, the linear decreasing region of the excess sorption as a function of bulk gas density can be investigated. The density at which this linear decreasing region has zero excess adsorption is equivalent to the density of the adsorbed layer. [Reference 23]

(xii) We conducted aberration corrected scanning transmission electron microscopy measurements at the ORNL Center for Nanophase Materials Sciences (Fig. 3). These show detailed atomic structure of synthetic carbon: demonstrating regions of graphitic and amorphous carbon consistent with 700 m^2/g BET surface areas. [References 16, 24]

(xiii) Pore conformability: we have performed a mechanical analysis of the stability of pores in carbon, this indicates that pores with lateral (in plane) dimensions larger than 2-4 nm would naturally collapse and close, consistent with our SAXS experiments. More interestingly, we observe that pores that are above this "critical length" may be partially opened by H_2 at P > 20-30 bar. See Fig. 6. This "opening of the pores" may have important consequences for the adsorption isotherms. In a realistic adsorbent comprised of a variety of small and large pores we would see the gradual filling of the open pores at low pressures. However, as the pressure increases, some of the closed pores may start open-

ing as described above. This causes the adsorption to raise faster than expected from the low-pressure data, and may explain the *anomalous* adsorption isotherms (maximum of excess adsorption absent, or shifted to very high pressures) observed in our polymer-based carbons. [Reference 23]

(xiv) The analysis of adsorbed films from isosteric heat determinations (Clausius-Clapeyron), gives film thicknesss of the sueprcritically adsorbed films of 4.1 Å and 6.1 Å, at 80 K and 303 K (Fig. 7, right). The corresponding film thicknesses are $\rho_{film} \leq 86$ g/L (80 K), 15 g/L (303 K). The 80 K density is significantly higher then bulk liquid density of 71 g/L of hydrogen at its normal boiling point, 20 K. Should this film density be associated to a gas phase (as suggested by bulk thermodyanmics, according to which no liquid state exists above the critical temperature, 33 K, for hydrogen) or a liquid (as suggested by the high density)? The answer is: it is a liquid because the film has a fixed volume independent of the size of the container ("a liquid maintains its volume"). Independent evidence of the assertion that the film is essentially incompressible comes from analysis of gravimetric excess adsorption as a function of the gas density (Fig. 7, left): (i) as the gas density is increased, the excess adsorption decays linearly, its extrapolation to $n_{exc} = 0$ yields an estimate of the saturated adsorbed film density; (ii) Ono-Kondo theory fits to the excess adsorption also indicate an incompressible film (not shown). Table 1 shows estimates of the film densities from the two models. The results are in remarkable agreement with the film densities from the Clausius-Clapeyron analysis. [Reference 15, 24]

(xv) We have also demonstrated the possibility of a new class of high-surface area carbon structures ("Open Carbon Frameworks"), which goes beyond the traditional model of parallel graphene sheets. The structures have locally planar units (unbounded or bounded fragments of graphene sheets),and variable ratios of in-plane to edge atoms. Adsorption of molecular hydrogen on these structures was studied by performing grand canonical Monte Carlo simulations with appropriately chosen adsorbent−adsorbate interaction potentials. These result in a rich spectrum of relationships between structural characteristics of carbons and ensuing hydrogen adsorption (structure−function relationships). In particular, storage capacities higher than in slit-shaped pores can be obtained by fragmentation/truncation of graphene sheets, which creates surface areas exceeding of 2600 m^2/g, the maximum surface area for infinite graphene sheets, carried mainly by edge sites. For OCFs with a ratio of in-plane to edge sites ≈ 1 and surface areas 3800−6500 m^2/g, we found record maximum excess adsorption of 75−85 g of H_2/kg of C at 77 K and record storage capacity of 100−260 g of H_2/kg of C at 77 K and 100 bar. See Fig. 8. [References 3, 4, 5, 19, 23]

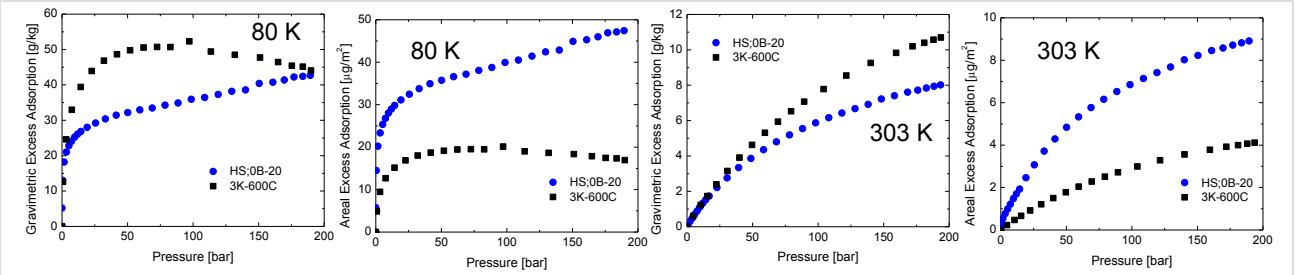

Figure 1. H_2 excess adsorption at 80 K and 303 K for synthetic carbon HS;0B-20 and graphene-like carbon 3K-600C. Areal excess adsorption (gravimetric excess adsorption divided by specific surface area, Σ_{BET}), Frame 2 and 4 from left, shows that the synthetic carbon has more than twice the number of hydrogen molecules adsorbed for surface area.

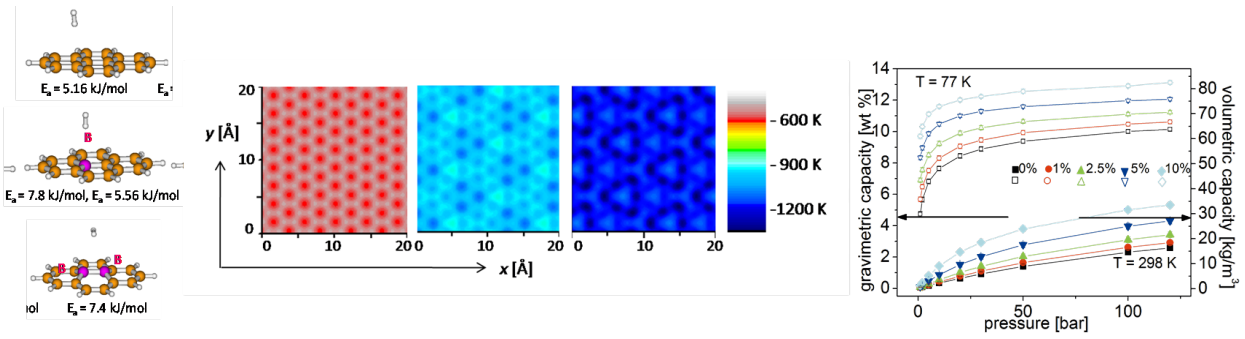

Figure. 2. Left: H_2 binding energy in boron-doped carbon (calculated at MP2 level). Center: Energy landscape for hydrogen adsorption on a single graphite sheet (E_{aver} = -590 K) (left), ~5% B:C (BC_{17}, E_{aver} = -930 K) (center) and ~11% B:C (BC_8, E_{aver} = -1180 K) (right) surfaces. The color scale is the same for all graphs. Right: Gravimetric (left axis) and volumetric (right axis) adsorption of hydrogen in graphene slit pores of width d = 1.2 nm as a function of pressure and the percentage of boron content in the pore wall, for T = 77 K and 298 K. For reference, the arrows indicate both gravimetric and volumetric US DOE targets required to be reached by 2010 by the storing system.

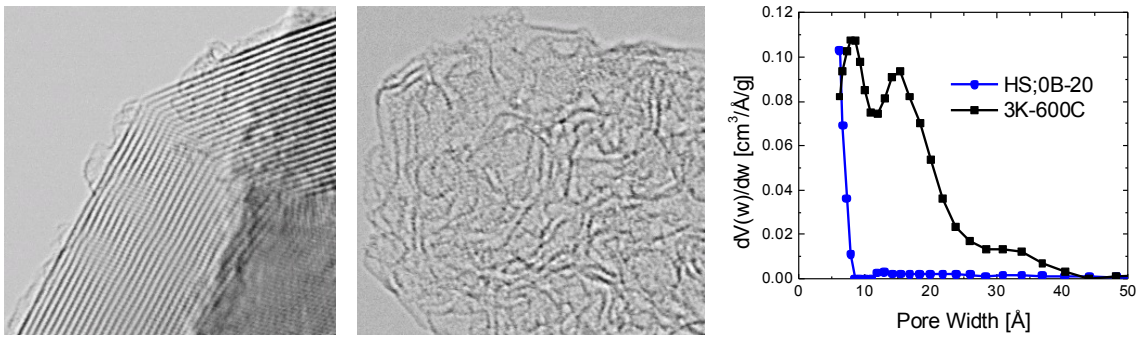

Figure 3. Left and center: High resolution transmission electron micrographs (Nion UltraSTEM, Oak Ridge National Laboratory) of U. Missouri PVDC-based carbon HS;0B-20. The distance between planes and between carbons in a plane is consistent with a distorted graphene/graphitic structure. Right: comparison of the pore size distribution of HS;0B-20 with that of a graphene-like activated carbon, U. Missouri sample 3K-600C. The PVDC carbon has a very narrow, monodisperse distribution centered around 0.6 nm. Surface areas, Σ_{BET}, and porosities, ϕ: HS;0B-20: Σ_{BET} = 900 m^2/g, porosity ϕ = 0.46, 3K-600C: Σ_{BET} = 2600 m^2/g, ϕ = 0.76.

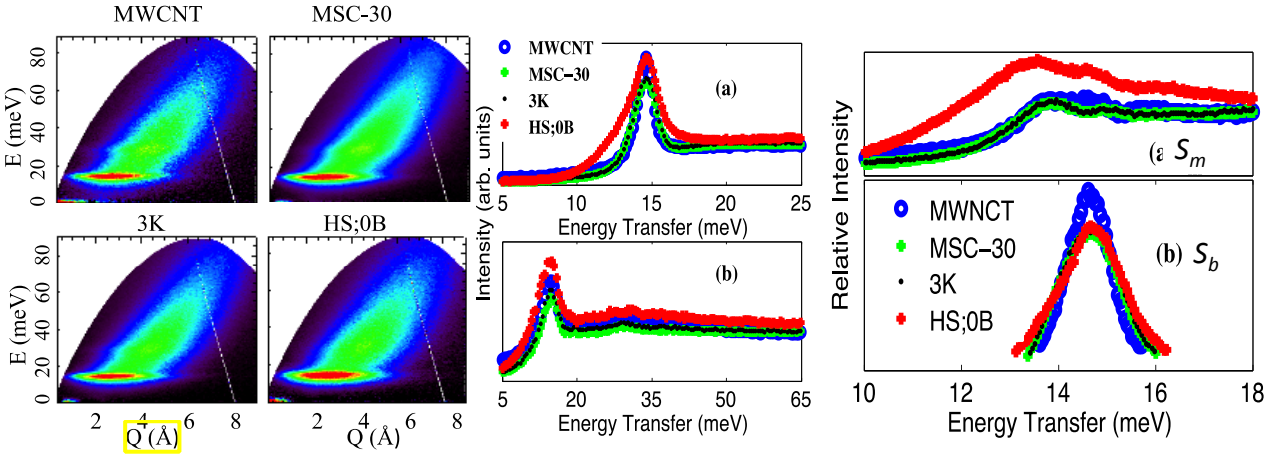

Figure 4. Left: IINS intensities for 4 carbons. Center: momentum-averaged spectra for 30 meV (top) and 90 meV (bottom) incident neutrons. Right: decomposition of the IINS spectra into localized and mobile components S_b and S_m. See Ref. [12].

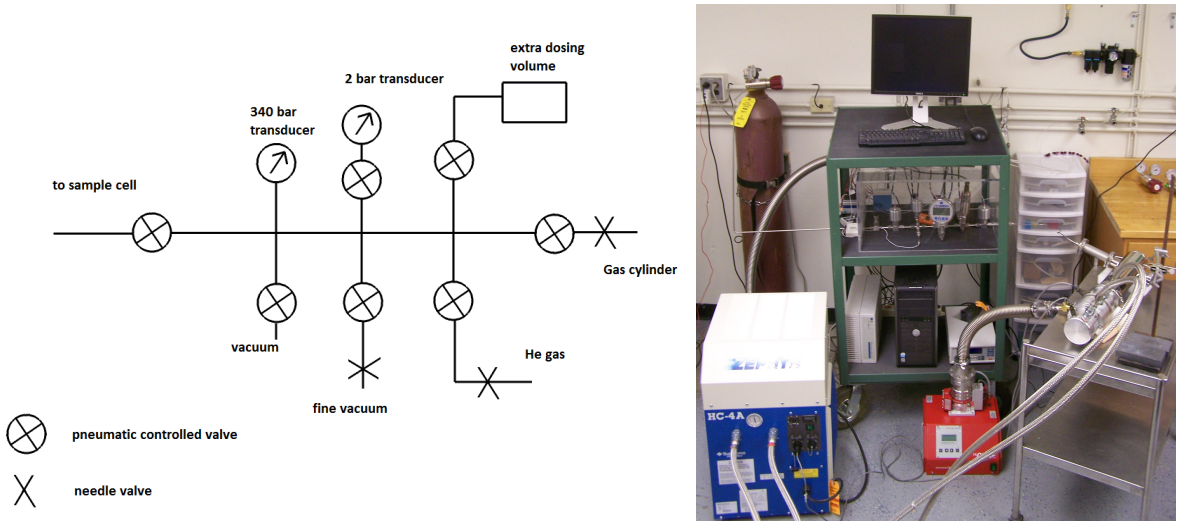

Figure 5. 20-K hydrogen sorption analyzer at the University of Missouri.

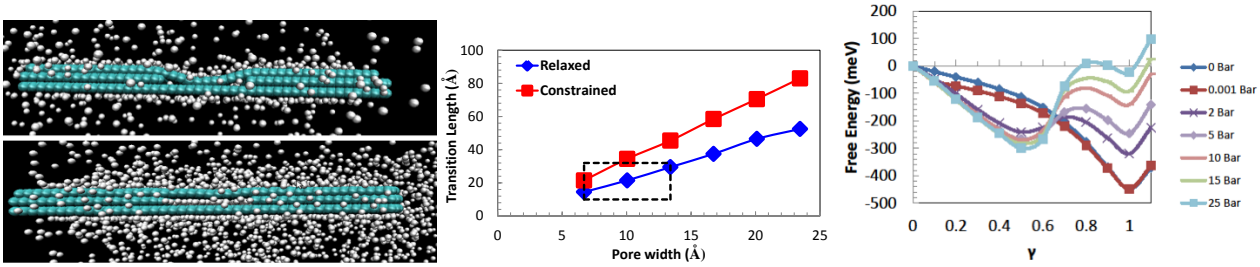

Figure 6. Left: a finite pore resulting from two graphene flakes partially intercalated. For large lateral dimensions, the pores are mechanically unstable and collapse (top). At higher pressures, adsorbed H_2 solvation forces are able to inflate the pores (bottom). Center: "critical pore length" vs. pore width resulting from minimization of the energy functional (3) for two extreme boundary conditions. The box indicates the region compatible with pore-size distributions determined from N_2 subcritical adsorption (horizontal axis), and SAXS analysis of lateral dimensions (vertical axis). Right: Free energy vs. generalized pore coordinate γ for a pore of $H = 7$ Å, $L = 20$ Å. Here γ = 0,1 represents a completely open, closed pore, respectively. For this H, L the pore opens at $P \sim 5$ bar as seen by the reduction of the free energy of the left local minimum. Right: isotherms for various γ. As the pressure increases the adsorption isotherms would gradually shift from the γ = 0 to γ = 0.5.

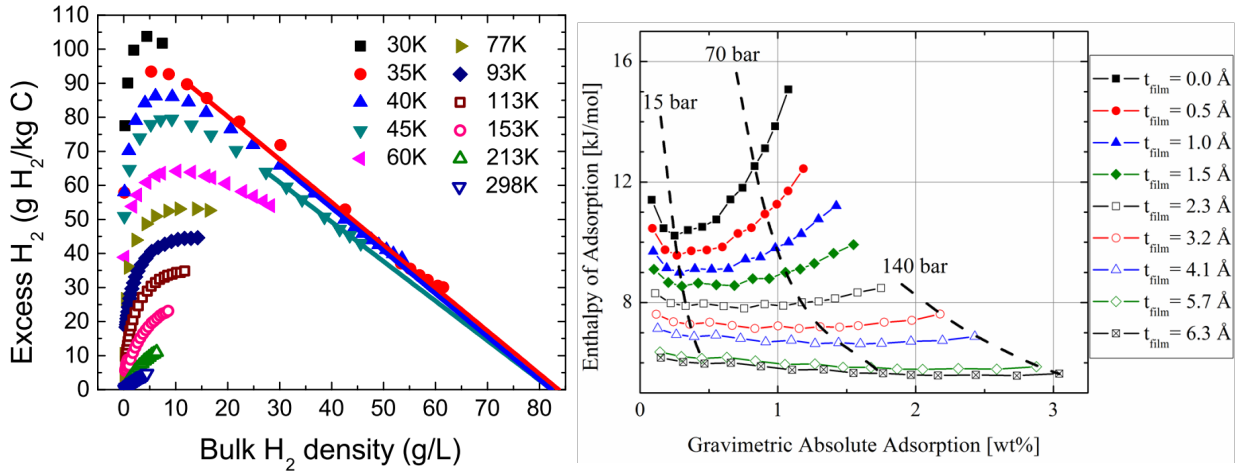

Figure 7. Determination of saturated film densities from extrapolation of the excess adsorption (left). Determination of film thicknesses (and volume) from the thermodynamic requirement that the isosteric heat of adsorption is a monotonically decreasing function of coverage (right). At the lower bound for film thickness, $t_{film} = 4.1$ Å, these results are consistent with the adsorption values.

Table 1. Ono-Kondo and linear extrapolation analyses of the film volumes and densities. For comparison, the Clausius-Clapeyron analysis yields $\rho_{film} \leq 86$ g/L (80 K), 15 g/L (303 K).

	Ono-Kondo		Linear extrapolation	
Temperature	Adsorbed film density (g/L)	Binding energy (kJ/mol)	Adsorbed film density (g/L)	Film thickness (Å)
35 K	82	1.6	84	4.5
40 K	83	1.6	82	4.5
45 K	81	1.7	82	4.9

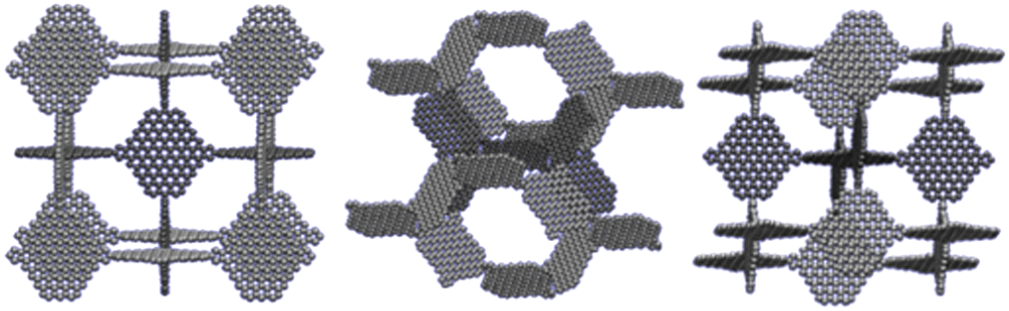

Figure 8. Open Carbon Frameworks

III - Publications & Presentations

a) Publications Acknowledging Support by DMSE (all peer reviewed)

1. *Quantum excitation spectrum of hydrogen adsorbed in nanoporous carbons observed by inelas- tic neutron scattering,* R. Olsen, M. Beckner, P. Pfeifer, **C. Wexler,** and H. Taub, Carbon **58,** 46- 58 (2013). Acknowledgement: This research was supported by the Department of Energy Office of Basic Energy Science (DOE- BES) under contract DE-FG02-07ER46411. Research at Oak Ridge National Laboratory's Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy. H.T. was supported by the National Science Foundation (NSF) under contract number DMR-0705974 and DGE-1069091. R.J.O. was also supported in part by the DOE Office of Energy Efficiency and Renewable Energy (EERE) Postdoctoral Research Awards under the EERE Fuel Cell Technologies Program, administered by the Oak Ridge Institute for Science and Education (ORISE) for the DOE. ORISE is managed by Oak Ridge Associated Universities (ORAU) under DOE contract number DEAC05- 06OR23100.
2. *Infrared study of boron–carbon chemical bonds in boron-doped activated carbon,* J. Romanos, D. Stalla, M. Beckner, A. Tekeei, G. Suppes, S. Jalisatgi, M. Lee, F. Hawthorne, D. Robertson, L. Firlej, B. Kuchta, C. Wexler, P. Yu, P. Pfeifer, Carbon **54,** 208-214 (2013). Acknowledgement: This work is supported by the United States Department of Energy Grants DE-FG02-07ER46411 and DE-FC36-08GO18142.
3. *Open carbon frameworks—a search for optimal geometry for hydrogen storage,* B. Kuchta, L. Firlej, A. Mohammadhosseini, M. Beckner, J. Romanos, and P. Pfeifer, "." *J. Mol. Mod.* **19,** 4079 (2013). Acknowledgement: This material is based upon work supported by the United States Department of Energy Grant No. DE-FG02-07ER46411.
4. *Increased H_2 gravimetric storage capacity in truncated slit pores modeled by grand canonical Monte Carlo simulations*. L. Firlej, B. Kuchta, A. Lazarewicz, and P. Pfeifer, *Carbon* **53**, 208-215 (2013). Acknowledgement: This material is based upon work supported by the United States Department of Energy Grant No. DE-FG02-07ER46411.
5. *Hypothetical high-surface-area carbons with exceptional hydrogen storage capacities: Open Carbon Frameworks*. B. Kuchta, L. Firlej, A. Mohammadhosseini, P. Boulet, M.W. Beckner, J. Romanos, and P. Pfeifer, *J. Am. Chem. Soc.* **134**, 15130-15137 (2012). Acknowledgement: This material is based upon

work supported by the United States Department of Energy Grant No. DE-FG02-07ER46411.

6. Sub-nanometer characterization of activated carbon by inelastic neutron scattering, R. Olsen, L. Firlej, B. Kuchta, H. Taub, P. Pfeifer, and C. Wexler, Carbon **49**, 1663-1671 (2011). Acknowledgement: This material is based upon work supported in part by the Department of Energy under Award No. DE-FG02-07ER46411 and the US Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. Work by H.T. was partially supported by the US National Science Foundation under Grant No. DMR-0705974.
7. *Numerical Analysis of Hydrogen Storage in Carbon Nanopores*, C. Wexler, R. Olsen, P. Pfeifer, B. Kuctha, L. Firlej, Sz. Roszak, in *Condensed Matter Theories* Vol. 25, Eds. E.V. Ludeña, R.F. Bishop, & P. Iza (Nova Science Publishers, 2011). Acknowledgement: This material is based upon work supported in part by the U.S. Department of Energy under Award Nos. DE-FG02-07ER46411 and DE-FG36-08GO18142. We acknowledge the University of Missouri Bioinformatics Consortium for the use of their computational facilities.
8. *Influence of Structural Heterogeneity of Nano-Porous Sorbent Walls on Hydrogen Storage*, B. Kuchta, L. Firlej, Sz. Roszak, P. Pfeifer, and C. Wexler, Appl. Surf. Sci. **256**, 5270–5274 (2010). Acknowledgement: This material is based on work supported in part by the Department of Energy under Award Nos. DE-FG02-07ER46411 and DE-FC36-08GO18142 (L.F., B.K., P.F., and C.W). We acknowledge the Wroclaw and Poznan Supercomputing and Networking Centers and University of Missouri Bioinformatics Consortium for the use of their computational facilities.
9. *Numerical Estimation of Hydrogen Storage Limits in Carbon Based Nanospaces*, B. Kuchta, L. Firlej, P. Pfeifer, and C. Wexler, C**a**rbon **48**, 223-231 (2010). Acknowledgement: This material is based upon work supported in part by the Department of Energy under Award No. DE-FG02-07ER46411.
10. *Structural and Energetic Factors in Designing a Nanoporous Sorbent for Hydrogen Storage*, B. Kuchta, L. Firlej, R. Cepel, P. Pfeifer, and C. Wexler, Colloids and Surfaces A: Physicochem. Eng. Aspects **357**, 61–66 (2010). Acknowledgement: This material is based upon work supported in part by the Department of Energy under Award Nos. DE-FG02-07ER46411 and DE-FC36-08GO18142. We acknowledge the University of Missouri Bioinformatics Consortium for the use of their computational facilities.
11. *Numerical Analysis of Hydrogen Storage in Carbon Nanopores*, C. Wexler, R. Olsen, P. Pfeifer, B. Kuctha, L. Firlej, Sz. Roszak, Int. J. Mod. Phys. B **24**, 5152-5162 (2010). Acknowledgement: This material is based upon work supported in part by the U.S. Department of Energy under Award Nos. DE-FG02-07ER46411 and DE-FG36-08GO18142. We acknowledge the University of Missouri Bioinformatics Consortium for the use of their computational facilities.
12. *Enhanced Hydrogen Adsorption in Boron Substituted Carbon Nanospaces*; L. Firlej, Sz. Roszak, B. Kuchta, P. Pfeifer, and C. Wexler, J. Chem. Phys. **131**, 164702 (2009). **Editor selection for the Vir. J. Nan. Sci. & Tech. 20, vol. 19 (2009).** Acknowledgement: This material is based on work supported in part by the Department of Energy under Award Nos. DE-FG02- 07ER46411 and DE-FC36-08GO18142 (L.F., B.K., P.F., and C.W.). We acknowledge the Wroclaw and Poznan Supercomputing and Networking Centers and University of Missouri Bioinformatics Consortium for the use of their computational facilities.
13. *Hydrogen Storage in Engineered Carbon Nanospaces*; J. Burress, M. Kraus, M. Beckner, R. Cepel, G. Suppes, C. Wexler, and P. Pfeifer; Nanotechnology **20**, 204026 (2009). **This publication was deemed "of great importance" by the reviewers and editors of the journal, and was featured on PhysOrg.com (http://www.physorg. com/news162195986.html).** Acknowledgement: This material is based upon work supported in part by the Department of Energy under Award No. DE-FG02-07ER46411. Use of the Advanced Photon Source was supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. CW and RC gratefully acknowledge the University of Missouri Bioinformatics Consortium for the use of their

computational facilities.

14. *Boron Substituted Graphene: Energy Landscape for Hydrogen Adsorption*; L. Firlej, B. Kuchta, C. Wexler, and P. Pfeifer; Adsorption **15**, 312-317 (2009). Acknowledgement: This material is based upon work supported in part by the Department of Energy under Award No. DE-FG02-07ER46411.
15. *Hydrogen Adsorption Studies of Engineered and Chemically Modified Activated Carbons*, M. Beckner, Ph.D. Dissertation (University of Missouri, 2012, P. Pfeifer, director).
16. *Nanospace Engineering of Porous Carbon For Gas Storage*, J. Romanos, Ph.D. Dissertation (University of Missouri, 2012, P. Pfeifer, director).
17. *Investigations of Novel Hydrogen Phenomena*, R. Olsen, Ph.D. Dissertation (University of Missouri, 2011,C. Wexler, director).
18. *Fundamental building blocks of nanoporous networks from ultra-small-angle x-ray scattering (USAXS) and small-angle x-ray scattering (SAXS) experiments*, M. Kraus, Ph.D. Dissertation (University of Missouri, 2010 P. Pfeifer, director).
19. *Different Approach to Estimation of Hydrogen-Binding Energy in Nanospace-Engineered Activated Carbons*. L. Firlej, M. Beckner, J. Romanos, P. Pfeifer, and B. Kuchta, J. Phys. Chem. C **118**, 955-961 (2014). Acknowledgement: This study is based on work supported by the Department of Energy Grant under award no. DE-FG02–07ER46411.
20. *Understanding universal adsorption limits for hydrogen storage in nanoporous systems*. L. Firlej, P. Pfeifer, and B. Kuchta, Adv. Mater. **25**, 5971-5974 (2013). Acknowledgement: This study is based on work supported by the Department of Energy Grant under award no. DE-FG02–07ER46411.
21. *High-Surface-Area Biocarbons for Reversible On-Board Storage of Natural Gas and Hydrogen* , P. Pfeifer, J.W. Burress, M.B. Wood, C.M. Lapilli, S.A. Barker, J.S. Pobst, R.J. Cepel, C. Wexler, P.S. Shah, M.J. Gordon, G.J. Suppes, S.P. Buckley, D.J. Radke, J. Ilavsky, A.C. Dillon, P.A. Parilla, M. Benham, and M.W. Roth, In: *Life Cycle Analysis for New Energy Conversion and Storage Systems*, eds. V.M Fthenakis, A.C. Dillon, and N. Savage, Mater. Res. Soc. Symp. Proc. **1041**, 1041-R02-02 (2008). Acknowledgement: This material is based upon work supported by the National Science Foundation under Grant Nos. PFI- 0438469 and DUE-0618459, U.S. Department of Energy under Award No. DE-FG02-07ER46411, U.S. Department of Defense under Award No. N00164-07-P-1306, U.S. Department of Education under Award No. P200A040038, University of Missouri (RB-06-40), and Midwest Research Institute. Acknowledgment is also made to the Donors of the American Chemical Society Petroleum Research Fund (PRF43277ñB5, M.W.R.). Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.
22. *High Surface Area Carbon and Process for Its Production,* P. Pfeifer, G.J. Suppes, P. Shah, and J.W. Burress, International Patent Application Published under the Patent Cooperation Treaty (PCT). International Application No. PCT/US2007/084061; International Publication No. WO 2008/058231. World International Property Organization (WIPO), Geneva, May 15, 2008.
23. *New Pathways and Metrics for Enhanced, Reversible Hydrogen Storage in Boron–Doped Carbon Nanospaces,* P. Pfeifer, C. Wexler, M.F. Hawthorne, M.W. Lee, and S. Jalisatgi, In: *DOE Hydrogen and Fuel Cells Program, 2012 Annual Progress Report*, ed. S. Satyapal (U.S. Department of Energy, Washington, DC, 2012; DOE/GO-102012-3767), p. IV-(233-235).
    http://www.hydrogen.energy.gov/annual_progress12.html
    http://www.hydrogen.energy.gov/pdfs/progress12/iv_h_7_pfeifer_2012.pdf
24. *Networks of Boron-Doped Carbon Nano-pores for Low-Pressure Reversible Hydrogen Storage,* P. Pfeifer, M.F. Hawthorne, and C. Wexler, In: *DOE Hydrogen Program, 2009 Annual Progress Report*, ed. S. Satyapal (U.S. Department of Energy, Washington, DC, 2009; DOE/GO-102009-2950), p. 824-829.
    http://www.hydrogen.energy.gov/annual_progress09.html
    http://www.hydrogen.energy.gov/pdfs/progress09/iv_i_6_pfeiffer.pdf
25. *Nature-Inspired Energy and Material Efficient Design of a Polymer Electrolyte Fuel Cell*, S. Kjelstrup, M.-O. Coppens, J. Pharoah, and P. Pfeifer, Energy Fuels **24**, 5097-5108 (2010). Acknowledgement: The

authors are grateful to the Center for Advanced Study at The Norwegian Academy of Science and Letters for extraordinary sabbatical stays. This material is also based upon work supported in part by the U.S. National Science Foundation under Grant DGE-0504361 (MOC) and the U.S. Department of Energy under Award DE-FG02-07ER46411 (PP)

26. *Nature-Inspired Design of a Polymer Electrolyte Fuel Cell,* S. Kjelstrup, M.-O. Coppens, J. Pharoah, and P. Pfeifer, In: *ECOS 2010—Proceedings of the 23rd International Conference on Efficiency, Cost, Optimization, Simulation, and Environmental Impact of Energy Systems* (École Polytechnique Fédéral de Lausanne, Lausanne, Switzerland, 2010). Acknowledgement: The authors are grateful to the Center for Advanced Study at The Norwegian Academy of Science and Letters for extraordinary sabbatical stays. This material is also based upon work supported in part by the U.S. National Science Foundation under Grant DGE-0504361 (MOC) and the U.S. Department of Energy under Award DE-FG02-07ER46411 (PP)

b) Conference Presentations and Talks in Colleges and Universities (*=invited, $^{\pi}$=poster):

1. **Modeling the adsorption-induced breathing of nanoporous carbon*, M.J. Connolly, C. Wexler, 7th NIST Workshop on Atomistic Simulations for Industrial Needs: Materials for Gas Separation Applications, Gaithersburg, MD, July/2014. **Invited talk presented by CW**
2. *Hydrogen densities greater than liquid hydrogen at 77 K in engineered carbon nanospaces*. P. Pfeifer, A. Gillespie, E. Dohnke, and Y. Soo, In: *Materials Challenges in Alter-native & Renewable Energy, Conference Program* (American Ceramic Society, Colum-bus, OH, 2014), MCARE-166-2014, p. 36. **Talk Presented by PP.**
3. **Adsorption-induced conformational changes in porous materials*, M.J. Connolly, C. Wexler, 10th International Symposium on the Characterization of Porous Solids (COPS-X), O34. Granada, Spain, May/2014. **Invited talk presented by CW**.
4. $^{\pi}$*Boron Doping of Activated Carbon*, M. J. Connolly, A. St. John, M. Beckner, P. Pfeifer, C. Wexler, University of Missouri, Columbia, MO/USA, 10th International Symposium on the Characterization of Porous Solids (COPS-X), B6. Granada, Spain, May/2014. **Poster presented by CW**.
5. *Adsorption-induced breathing in nanoporous carbon*, M. Connolly, C. Wexler, *Bull. Am. Phys. Soc.* **59**, Z37.00011 (2014). Denver, CO, Mar/2014. **Talk Presented by MC.**
6. *Energetics of Boron Doping of Carbon Pores*, *Bull. Am. Phys. Soc.* **59**, Z37.00007 (2014). Denver, CO, Mar/2014. **Talk Presented by MC.**
7. *Adsorption-Induced Conformational Changes in Porous Materials,* M. Connolly, C. Wexler, American Physical Society Prairie Section Meeting C2.00002 (2013). Columbia, MO, Nov/2013. **Talk Presented by MC.**
8. $^{\pi}$*Boron Doping of Activated Carbon,* M. Connolly, A. St. John, M. Beckner, P. Pfeifer, C. Wexler, American Physical Society Prairie Section Meeting F1.00010 (2013). Columbia, MO, Nov/2013. **Poster presented by MC**.
9. **Adsorbate-induced Breathing of Nanoporous Carbon*, M. Connolly, J. Burress, C. Wexler, 11th International Conference on the Fundamentals of Adsorption (FOA-11), L-306. Baltimore, MD, May/2013. **Invited talk presented by CW.**
10. *Measurement of increased enthalpies of adsorption for boron-doped activated carbons*. A. Gillespie, M. Beckner, N. Chada, J. Schaeperkoetter, A. Singh, M. Lee, C. Wexler, J. Burress, and P. Pfeifer, *Bull. Am. Phys. Soc.* **58**, M38.00010 (2013). Baltimore, MD, Mar/2013. **Talk Presented by AG.**
11. *Adsorbed Hydrogen Film Densities and Thicknesses Determined from Low-Temperature Hydrogen Sorption Experiments*, J. Burress, E. Dohnke, M. Beckner, M. Lee, C. Wexler, P. Pfeifer, *Bull. Am. Phys. Soc.* **58**, M38.00008 (2013). Baltimore, MD, Mar/2013. **Talk Presented by ED.**
12. **Doping activated carbon for hydrogen storage*, C. Wexler, 1st Iberoamerican Symposium on Adsorption, Recife, Brasil, May, 2012. **Invited talk presented by CW**.
13. *Conformability of Pores in Activated Carbon*, M. Connolly and C. Wexler, 1st Iberoamerican Symposi-

um on Adsorption, Recife, Brasil, May, 2012. **Poster presented by CW**.

14. *Elastic Pore Structure of Activated Carbon*, M. Connolly and C. Wexler, The 6th International Workshop on Characterization of Porous Materials–from Angstroms to Millimeters (CPM-6), Delray Beach, FL, April, 2012. **Poster presented by MC**.
15. *Recoiling and Bound Quantum Excitations of Adsorbed Hydrogen As An Assessment of Planarity*, R. Olsen, H. Taub and C. Wexler, The 6th International Workshop on Characterization of Porous Materials–from Angstroms to Millimeters (CPM-6), Delray Beach, FL, April, 2012. **Poster presented by RO**.
16. *Reversible Storage of Hydrogen and Natural Gas in Nanospace-Engineered Activated Carbons*, J. Romanos, M. Beckner, T. Rash, P. Yu, G. Suppes, and P. Pfeifer, *March 2012 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **57**, W33.05 (2012)), Boston, MA, March 2012. **Talk Presented by JR.**
17. *Measured Enthalpies of Adsorption of Boron-Doped Activated Carbons*, M. Beckner, J. Romanos, E. Dohnke, A. Singh, J. Schaeperkoetter, D. Stalla, J. Burress, S. Jalisatgi, G. Suppes, M. F. Hawthorne, P. Yu, C. Wexler, and P. Pfeifer, *March 2012 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **57**, W33.07 (2012)), Boston, MA, March 2012. **Talk Presented by MB.**
18. *Performance of Carbon Hydrogen Storage Materials as a Function of Post-Production Thermal Treatment*, E. Dohnke, J. Romanos, M. Beckner, J. Burress, P. Yu, and P. Pfeifer, *March 2012 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **57**, W33.08 (2012)), Boston, MA, March 2012. **Talk Presented by ED.**
19. *The Stationary States of Adsorbed Hydrogen*, R. Olsen, H. Taub, and C. Wexler, *March 2012 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **57**, W33.06 (2012)), Boston, MA, March 2012. **Talk Presented by RO.**
20. *Measured Enthalpies of Adsorption of Boron-Doped Activated Carbons*, M. Beckner, J. Romanos, E. Dohnke, A. Singh, J. Schaeperkoetter, D. Stalla, J. Burress, S. Jalisatgi, G. Suppes, M.F. Hawthorne, P. Yu, C. Wexler, and P. Pfeifer, *March 2012 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **57**, W33.07 (2012)), Boston, MA, March 2012. **Talk Presented by MB.**
21. *Adsorption-induced Pore Expansion and Contraction in Activated Carbon*, M. Connolly and C. Wexler, *March 2012 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **57**, X11.11 (2012)), Boston, MA, March 2012. **Talk Presented by MC.**
22. **Nanoporous Carbon for Reversible Storage of Hydrogen*, C. Wexler, *Low Carbon Earth Summit-2011 (LCES-2011)*, Dalian, China, October 2011. **Invited talk presented by CW**.
23. **The Quantum Excitation Spectrum of Adsorbed Hydrogen*, R. Olsen, International Workshop: Adsorption at the Nanoscale, a New Frontier in Fundamental Science & Applications, Columbia, MO, September 2011. **Invited talk presented by RO.**
24. **Open Carbon Frameworks (OCF) – new hypothetical structures for hydrogen storage*, B. Kuchta, International Workshop: Adsorption at the Nanoscale, a New Frontier in Fundamental Science & Applications, Columbia, MO, September 2011. **Invited talk presented by BK.**
25. **Influence of edges on adsorption in nanopores with finite pore walls from truncated graphene*, L. Firlej, International Workshop: Adsorption at the Nanoscale, a New Frontier in Fundamental Science & Applications, Columbia, MO, September 2011. **Invited talk presented by LF.**
26. **Nanospace-Engineered Carbons for Reversible On-Board Storage of Natural Gas and Hydrogen*, J. Romanos, International Workshop: Adsorption at the Nanoscale, a New Frontier in Fundamental Science & Applications, Columbia, MO, September 2011. **Invited talk presented by JR.**
27. *Analysis of hydrogen sorption characteristics of boron-doped activated carbons*, M. Beckner, International Workshop: Adsorption at the Nanoscale, a New Frontier in Fundamental Science & Applications, Columbia, MO, September 2011. **Poster presented by MB.**
28. *Flexible Pore Walls in Activated Carbon*, M. Connolly, International Workshop: Adsorption at the Nanoscale, a New Frontier in Fundamental Science & Applications, Columbia, MO, September 2011. **Poster presented by MC.**
29. *The effect of KOH:C and activation temperature on hydrogen storage capacities of activated carbons*, T. Rash, International Workshop: Adsorption at the Nanoscale, a New Frontier in Fundamental Science & Applications, Columbia, MO, September 2011. **Poster presented by TR.**

30. *Boron-neutron Capture on Activated Carbon for Hydrogen Storage*, J. Romanos, International Workshop: Adsorption at the Nanoscale, a New Frontier in Fundamental Science & Applications, Columbia, MO, September 2011. **Poster presented by JR.**
31. *A high volume, high throughput volumetric sorption analyzer*, Y. Soo, International Workshop: Adsorption at the Nanoscale, a New Frontier in Fundamental Science & Applications, Columbia, MO, September 2011. **Poster presented by TR.**
32. *Nanopore structure from small angle and ultra-small angle x-ray scattering in engineered activated carbons for hydrogen storage*, D. Stalla, International Workshop: Adsorption at the Nanoscale, a New Frontier in Fundamental Science & Applications, Columbia, MO, September 2011. **Poster presented by DS.**
33. *Inelastic Neutron Scattering from Hydrogen Adsorbed in Carbon*, C. Wexler, R. Olsen, H. Taub, P. Pfeifer, M. Beckner, Gordon Research Conference "Nanoporous Materials & Their Applications", Holderness, NH, August 2011. **Poster presented by CW.**
34. **Characterization of activated carbon at the sub-nm scale via adsorption (H_2, N_2, CH_4, isosteric heats), TEM, FT-IR, neutron (IINS) and x-ray (SAXS/USAXS); and application towards optimization of H_2 storage*, C. Wexler, P. Pfeifer, M. Kraus, M. Beckner, J. Romanos, D. Stalla, T. Rash, H. Taub, P. Yu, R. Olsen, and J. Ilavsky, 9th International Symposium on the Characterisation of Porous Solids (COPS 9), DECHEMA (*Gesellschaft für Chemische Technik und Biotechnologie e.V.*), Dresden, Germany, June 2011. **Invited talk presented by CW**.
35. *Inelastic neutron scattering from adsorbed hydrogen*, R. Olsen, M. Beckner, C. Wexler, H. Taub and P. Pfeifer, Wilhelm and Else Heraeus Seminar: Energy Materials Research by Neutrons and Synchrotron Radiation, Bad Honnef, Germany, May 2011. **Poster presented by RO.**
36. *Nanopore structure from small angle and ultra-small angle x-ray scattering in engineered activated carbons for hydrogen storage*, D. Stalla, M. Kraus, J. Romanos, M. Beckner, J. Ilavsky, C. Wexler, and P. Pfeifer, Wilhelm and Else Heraeus Seminar: Energy Materials Research by Neutrons and Synchrotron Radiation, Bad Honnef, Germany, May 2011. **Poster presented by DS.**
37. **A Nanoporous Carbon "Sponge" for Hydrogen Storage*, C. Wexler, Physics Colloquium, University of Buffalo, Buffalo, NY, April 2011. **Invited talk presented by CW**.
38. *Insights on the pore structure of activated carbon*, M. Connolly and C. Wexler, *USC-Department of Energy Conference on Materials for Energy Applications—Experiment, Modeling and Simulations,* Terranea, CA, April 2011. **Poster presented by MC.**
39. *Anomalous Characteristics of a PVDC Carbon Adsorbant*, C. Wexler, M. Beckner, J. Romanos, T. Rash, P. Pfeifer, and R. Olsen, *March 2011 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **56**, H20.09 (2011)), Dallas, TX, March 2011. **Contributed talk presented by RO.**
40. *Evaluation of the isosteric heat of adsorption at zero coverage for hydrogen on activated carbons*, E. Dohnke, M. Beckner, J. Romanos, R. Olsen, C. Wexler, And P. Pfeifer, *March 2011 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **56**, H20.10 (2011)), Dallas, TX, March 2011. **Contributed talk presented by MB.**
41. *Inelastic Neutron Scattering from Hydrogen Adsorbed in Carbon*, R. Olsen, M. Beckner, P. Pfeifer, and C. Wexler, *March 2011 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **56**, H20.11 (2011)), Dallas, TX, March 2011. **Contributed talk presented by RO.**
42. *Analysis of hydrogen sorption characteristics of boron-doped activated carbons* M. Beckner, J. Romanos, D. Stalla, E. Dohnke, A. Singh, M. Lee, G. Suppes, M.F. Hawthorne, P. Yu, C. Wexler, and P. Pfeifer, *March 2011 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **56**, H20.12 (2011)), Dallas, TX, March 2011. **Contributed talk presented by MB.**
43. *The effect of KOH:C and activation temperature on hydrogen storage capacities of activated carbons,* T. Rash, M. Beckner, J. Romanos, E. Leimkuehler, A. Tekeei, G. Suppes, C. Wexler, and P. Pfeifer*, March 2011 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **56**, H20.13 (2011)), Dallas, TX, March 2011. **Contributed talk presented by TR.**
44. *Opening of slit-shaped pores from bending of graphene walls*, M. Connolly and C. Wexler, *March 2011 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **56**, T31.11 (2011)), Dallas, TX, March

2011. **Contributed talk presented by MC.**

45. *A high volume, high throughput volumetric sorption analyzer*, Y.C. Soo, M. Beckner, J. Romanos, C. Wexler, and P. Pfeifer, *March 2011 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **56**, V20.03 (2010)), Dallas, TX, March 2011. **Contributed talk presented by YS.**
46. **Explaining the Hydrogen Adsorption of a Carbon Adsorbant Manufactured by the Pyrolosis of Saran*, R. Olsen and C. Wexler, Physics Colloquium, University of Northern Iowa, Cedar Falls, IA, January 2011. **Invited talk presented by RO.**
47. *Inelastic Neutron Scattering from Adsorbed Hydrogen*, R. Olsen, M. Beckner, H. Taub, and C. Wexler, Fall 2010 Meeting of the Prairie Section of the American Physical Society, Chicago, IL, November 2010. **Contributed talk presented by RO.**
48. **A Brief History of Energy*, C. Wexler, Global Issues Colloquium (Public Lecture), C. Wexler Truman State University, Kirksville, MO, September 2010. **Invited public lecture presented by CW.**
49. **Adsorption of Hydrogen in Boron Substituted Carbon-Based Porous Materials*, L. Firlej, B. Kuchta, P. Pfeifer, and C. Wexler, *10th International Conference on Fundamentals of Adsorption (FOA10)*, Awaji, Hyogo, Japan, May 2010. **Invited talk presented by LF.**
50. *Characterization of Sub-nm Pores in Carbon by Inelastic Neutron Scattering*, R. Olsen, B. Kuchta, L. Firlej, P. Pfeifer, H. Taub, and C. Wexler, *10th International Conference on Fundamentals of Adsorption (FOA10)*, Awaji, Hyogo, Japan, May 2010. **Poster presented by CW.**
51. *High Storage Capacity of Hydrogen in Heterogeneous Carbon Nanopores: Experimental, Theoretical and Computational Characterization*, C. Wexler, R. Olsen, M. Kraus, M. Beckner, B. Kuchta, L. Firlej, and P. Pfeifer, *10th International Conference on Fundamentals of Adsorption (FOA10)*, Awaji, Hyogo, Japan, May 2010. **Poster presented by CW.**
52. **Engineering a Nanoporous "Sponge" for Hydrogen Storage*, C. Wexler, Colloquium, Department of Physics, University of Vermont, Burlington, VT, April 2010. **Invited talk presented by CW.**
53. **Hydrogen Absorption in Nanoporous Carbon*, C. Wexler, Condensed Matter Seminar, Washingtong University, St. Louis, MO, April 2010. **Invited talk presented by CW.**
54. **A Brief History of Energy*, C. Wexler, Public lecture in *Saturday Morning Science* (http://satscience.missouri.edu), Columbia, MO, February 2010. **Invited public lecture presented by CW.**
55. *Record Hydrogen Storage Capacities in Advanced Carbon Storage Materials*, C. Wexler, M. Beckner, J. Romanos, J. Burress, M. Kraus, R. Olsen, E. Dohnke, S. Carter, G. Casteel, B. Kuchta, L. Firlej, E. Leimkuehler, A. Tekeei, G. Suppes, and P. Pfeifer, *March 2010 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **55**, T30.07 (2010)), Portland, OR, March 2010. **Contributed talk presented by MB.**
56. *Adsorption of Hydrogen in Boron-Substituted Nanoporous Carbons*, L. Firlej, B. Kuchta, Ss. Roszak, P. Pfeifer, and C. Wexler, *March 2010 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **55**, T30.09 (2010)), Portland, OR, March 2010. **Contributed talk presented by CW.**
57. *Isosteric Heats of Adsorption for Activated Carbons Made from Corn Cob*, M. Beckner, R. Olsen, J. Romanos, J. Burress, E. Dohnke, S. Carter, G. Casteel, C. Wexler, and P. Pfeifer, *March 2010 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **55**, T30.10 (2010)), Portland, OR, March 2010. **Contributed talk presented by RO and MB.**
58. *Quantization of Adsorbed Hydrogen for Inhomogeneous Materials Characterization using Inelastic Neutron Scattering*, R. J. Olsen, L. Firlej, B. Kuchta, P. Pfeifer, H. Taub, and C. Wexler, *March 2010 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **55**, T30.11 (2010)), Portland, OR, March 2010. **Contributed talk presented by RO.**
59. *Nanopore Structure from USAXS/SAXS in Advanced Carbon Materials for Hydrogen Storage*, M. Kraus, J. Ilavsky, M. Beckner, D. Stalla, C. Wexler, and P. Pfeifer, *March 2010 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **55**, T30.12 (2010)), Portland, OR, March 2010. **Contributed talk pre-**

sented by MK.

60. *Fractal Analysis of Boron Doped Activated Carbon*, M. Kraus, C. Wexler, and P. Pfeifer, *March 2010 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **55**, T30.13 (2010)), Portland, OR, March 2010. **Contributed talk presented by MK.**
61. *Structural and Energetic Factors in Designing a Perfect Nano-Porous Sorbent for Hydrogen Storage*, B. Kuchta, L. Firlej, R. Cepel, P. Pfeifer, and C. Wexler, The Missouri Nano Frontiers, Columbia, MO, November 2009. **Poster presented by BK.**
62. *Quantum Energy Levels of Hydrogen Adsorbed on Nanoporous Carbons*, R. Cepel, B. Kuchta, L. Firlej, P. Pfeifer, and C. Wexler, The Missouri Nano Frontiers, Columbia, MO, November 2009. **Poster presented by RC.**
63. **Hydrogen storage in engineered carbon nanospaces*, C. Wexler, The 2009 Physics Leaders Meeting, Department of Physics, University of Missouri, Columbia, MO, October 2009. **Invited talk presented by CW.**
64. *C. Wexler, R. Cepel, B. Kuchta, L. Firlej, and P. Pfeifer, "Theoretical approaches to hydrogen storage in nanoporous materials," In "33rd International Workshop on Condensed Matter Theories, CMT 33 (http://cmt33.senacyt.gov.ec), Quito, Ecuador, in August 16-22, 2009. **Invited talk presented by C. Wexler**.
65. *C. Wexler, "A Brief History of Alternative Energies." Opening (Public) Lecture In "33rd International Workshop on Condensed Matter Theories, CMT 33 (http://cmt33.senacyt.gov.ec), Quito, Ecuador, in August 16-22, 2009. **Invited public lecture presented by C. Wexler**.
66. *C. Wexler, "Breve Historia de las Energías Alternativeas: de la Leña al Hidrógeno(A Brief History of Alternative Energies: From Firewood to Hydrogen)," opening lecture to the *Taller de Energías Alternativas: Aportes a la Matriz Energética (Alternative Energies Workshop: Contributing Towards the Energy Infrastructure)*, Quito, Ecuador, August 2009. **Invited talk presented by C. Wexler.**
67. *B. Kuchta, L. Firlej, R.Cepel, C. Wexler and P. Pfeifer, "Influence of structural heterogeneity of nanoporous sorbent walls on hydrogen storage," The Seventh International Symposium Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids - ISSHAC-7 (http://www.isshac.org/), 5-11 July 2009, Kazimierz Dolny, Poland. **Invited talk presented by B. Kuchta**.
68. *C. Wexler, J. Burress, R. Cepel, B. Kuchta, L. Firlej, and P. Pfeifer, "Hydrogen storage in engineered carbon nanospaces: experimental results and theoretical/computional analysis," The Seventh International Symposium Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids - ISSHAC-7 (http://www.isshac.org/), 5-11 July 2009, Kazimierz Dolny, Poland. **Invited talk presented by B. Kuchta**.
69. B. Kuchta, L. Firlej, R.Cepel, C. Wexler, and P. Pfeifer, "Structural and Energetic Factors in Designing a Perfect Nano-porous Sorbent for Hydrogen Storage." In: *5th International Workshop on Characterization of Porous Materials from Angstroms to Milimeters*, New Brunswick, NJ, June 26-26, 2009 (http://porousmaterials.rutgers.edu). **Talk presented by B. Kuchta.**
70. P. Pfeifer, M. Kraus, J. Burress, M. Beckner, and C. Wexler, "Hierarchical Pore Structure Analysis of Engineered Carbon Nanospaces." In: *5th International Workshop on Characterization of Porous Materials from Angstroms to Milimeters*, New Brunswick, NJ, June 26-26, 2009 (http://porousmaterials.rutgers.edu). **Talk presented by M. Kraus.**
71. P. Pfeifer, J. Burress, M. Beckner, N. Kullman, R. Cepel, and C. Wexler, "Analysis of Hydrogen Adsorption Isotherms in Engineered Carbon Nanospaces." In: *5th International Workshop on Characterization of Porous Materials from Angstroms to Milimeters*, New Brunswick, NJ, June 26-26, 2009 (http://porousmaterials.rutgers.edu). **Poster presented by M. Kraus.**
72. C. Wexler, R. Cepel, B. Kuctha, L. Firlej, and P. Pfeifer, "Quantum Energy Levels of Hydrogen Adsorbed on Nanoporous Carbons." In: *5th International Workshop on Characterization of Porous Materi-*

als from Angstroms to Milimeters, New Brunswick, NJ, June 26-26, 2009 (http://porousmaterials.rutgers.edu). **Poster presented by B. Kuchta.**

73. *****P. Pfeifer, "Alliance for Collaborative Research in Alternative Fuel Technology (ALL-CRAFT)." In: *The Missouri Energy Summit, Columbia, MO, April 22-23, 2009. Scientific Program and Abstracts.* https://mospace.umsystem.edu/xmlui/handle/10355/514. **Invited talk presented by P. Pfeifer.**
74. *****C. Wexler, "Hydrogen Storage for Transportation." In *Physics Colloquium at the University of Northern Iowa*, February 18, 2009. **Invited talk presented by C. Wexler.**
75. R. Cepel, B. Kuchta, L. Firlej, P. Pfeifer, and C. Wexler, "Quantum energy levels of hydrogen adsorbed on nanoporous carbons: an intrinsic probe for pore structure, and improving Monte Carlo simulations of adsorption." In: *The Missouri Energy Summit, Columbia, MO, April 22-23, 2009. Scientific Program and Abstracts.* https://mospace.umsystem.edu/xmlui/handle/10355/962. **Poster presented by R. Cepel and C. Wexler**.
76. B. Kuchta, L. Firlej, R. Cepel, C. Wexler, and P. Pfeifer, "Structural and energetic factors in designing a perfect nano-porous sorbent for hydrogen storage." In: *The Missouri Energy Summit, Columbia, MO, April 22-23, 2009. Scientific Program and Abstracts.* https://mospace.umsystem.edu/xmlui/handle/10355/961. **Poster presented by B. Kuchta and C. Wexler**.
77. M. Beckner, J. Burress, C. Wexler, Z. Yang, F. Hawthorne, and P. Pfeifer, "Boron-Doped Carbon Nanospaces for High-Capacity Hydrogen Storage." *Bull. Am. Phys. Soc.* **54**, W27.00010 (2009). http://meetings.aps.org/Meeting/MAR09/Event/99321. **Talk presented by M. Beckner**—Session W27. *March 2009 Meeting of the American Physical Society*, Pittsburgh, PA, March 16-20 2009.
78. M. Kraus, J. Burress, M. Beckner, C. Wexler, and P. Pfeifer, "Hierarchical Pore Structure of Engineered Carbon Nanospaces for Use in Hydrogen Storage." *Bull. Am. Phys. Soc.* **54**, W27.00011 (2009). http://meetings.aps.org/Meeting/MAR09/Event/99322. **Talk presented by M. Beckner**—Session W27. *March 2009 Meeting of the American Physical Society*, Pittsburgh, PA, March 16-20 2009.
79. J. Burress, M. Beckner, N. Kullman, R. Cepel, C. Wexler, and P. Pfeifer, *Bull. Am. Phys. Soc.* **54**, W27.00012 (2009). http://meetings.aps.org/Meeting/MAR09/Event/99323. **Talk presented by J. Burress**—Session W27. *March 2009 Meeting of the American Physical Society*, Pittsburgh, PA, March 16-20 2009.
80. Raina Cepel, Bogdan Kuchta, Lucyna Firlej, Peter Pfeifer, and Carlos Wexler, "Quantum energy levels of hydrogen adsorbed on nanoporous carbons: an intrinsic probe for pore structure, and improving Monte Carlo simulations of adsorption." *Bull. Am. Phys. Soc.* **54**, W27.00013 (2009). http://meetings.aps.org/Meeting/MAR09/Event/99324. **Talk presented by R. Cepel**—Session W27. *March 2009 Meeting of the American Physical Society*, Pittsburgh, PA, March 16-20 2009.
81. B. Kuchta, L. Firlej, R. Cepel, C. Wexler, and P. Pfeifer, "Structural and energetic factors in designing a perfect nano-porous sorbent for hydrogen storage." *Bull. Am. Phys. Soc.* **54**, W27.00014 (2009). http://meetings.aps.org/Meeting/MAR09/Event/99325. **Talk presented by C. Wexler**—Session W27. *March 2009 Meeting of the American Physical Society*, Pittsburgh, PA, March 16-20 2009.
82. M. Wood, J. Burress, J. Pobst, S. Carter, P. Pfeifer, C. Wexler, P. Shah, and G. Suppes, "Structure of Nanoporous Biocarbon for Hydrogen Storage as Determined by Small-Angle X-Ray Scattering." *Bull. Am. Phys. Soc.* **53**, S36.00009 (2008). http://meetings.aps.org/Meeting/MAR08/Event/79881. **Talk presented by M. Wood**—Session S36: Focus Session: Hydrogen Storage III: Novel Porous and Sorption Materials. March 2008 Meeting of the American Physical Society, New Orleans, LA, March 10-14, 2008.
83. J. Burress, M. Wood, M. Gordon, P. Parilla, M. Benham, C. Wexler, F. Hawthorne, and P. Pfeifer, "High-Capacity Hydrogen Storage on Nanoporous Biocarbon." *Bull. Am. Phys. Soc.* **53**, S36.00010 (2008). http://meetings.aps.org/Meeting/MAR08/Event/79882. **Talk presented by J. Burress**—

Session S36: Focus Session: Hydrogen Storage III: Novel Porous and Sorption Materials. March 2008 Meeting of the American Physical Society, New Orleans, LA, March 10-14, 2008.

84. J. Pobst, J. Burresss, M. Wood, M. Beckner, P. Shah, M. Gordon, P. Parilla, S. Barker, S. Carter, L. Aston, G. Suppes, and P. Pfeifer, "Fabrication Procedures and Material Properties of Activated Carbon for Hydrogen and Methane Storage." *Bull. Am. Phys. Soc.* **53**, S36.00013 (2008). http://meetings.aps.org/Meeting/MAR08/Event/79885. **Talk presented by J. Pobst**—Session S36: Focus Session: Hydrogen Storage III: Novel Porous and Sorption Materials. March 2008 Meeting of the American Physical Society, New Orleans, LA, March 10-14, 2008.
85. R. Cepel, M. Beckner, C. Wexler, and P. Pfeifer. "Determination of Best Models for Adsorption of Hydrogen in Boron-Doped Carbon Nanopores." *Bull. Am. Phys. Soc.* **53**, U35.00002 (2008). http://meetings.aps.org/Meeting/MAR08/Event/80332. **Talk presented by R. Cepel**—Session U35: Focus Session: Hydrogen Storage IV: Theoretical Predictions. March 2008 Meeting of the American Physical Society, New Orleans, LA, March 10-14, 2008.
86. M.W. Roth, M.J. Connolly, P.A.Gray, and C. Wexler, "Molecular dynamics simulations of hexane on graphite at various coverages: the difference explicit hydrogens make." *Bull. Am. Phys. Soc.* **53**, V20.00010 (2008). http://meetings.aps.org/Meeting/MAR08/Event/80633. **Talk presented by M.J. Connolly**—Session V20: Phase Transitions: Structural, Electronic, and Magnetic. March 2008 Meeting of the American Physical Society, New Orleans, LA, March 10-14, 2008.
87. L. Firlej, B. Kuchta, M.W. Roth, Paul A. Gray, and Carlos Wexler. "Molecular Dynamics study of tetracosane monolayers adsorbed on graphite." *Bull. Am. Phys. Soc.* **53**, V20.00011 (2008). http://meetings.aps.org/Meeting/MAR08/Event/80634. **Talk presented by C. Wexler**—Session V20: Phase Transitions: Structural, Electronic, and Magnetic. March 2008 Meeting of the American Physical Society, New Orleans, LA, March 10-14, 2008.
88. B. Kuchta, L. Firlej, M.W. Roth, P.A. Gray, and C. Wexler, "Test of the universality of the scaling energy in alkanes using melting transition of layer adsorbed on graphite." *Bull. Am. Phys. Soc.* **53**, V20.00012 (2008). http://meetings.aps.org/Meeting/MAR08/Event/80635. **Talk presented by C. Wexler**—Session V20: Phase Transitions: Structural, Electronic, and Magnetic. March 2008 Meeting of the American Physical Society, New Orleans, LA, March 10-14, 2008.
89. O. Ciftja and C. Wexler, "Anisotropy in two-dimensional electronic quantum Hall systems at half filling of valence Landau levels." *Bull. Am. Phys. Soc.* **53**, V37.00011 (2008). http://meetings.aps.org/Meeting/MAR08/Event/80854. **Talk presented by C. Wexler**—Session V37: QHE and FQHE. March 2008 Meeting of the American Physical Society, New Orleans, LA, March 10-14, 2008.
90. *Mikael Wood, Jacob Burress, Peter Pfeifer, Carlos Wexler, Jan Ilavsky, "The Structure of Nanoporous Biocarbon for Hydrogen Storage as Determined by Small-Angle X-ray Scattering." In: *Users Week 2008, Advanced Photon Source, Argonne National Laboratory, May 4-8, 2008. Book of Abstracts (Argonne National Laboratory, 2008).* http://www.aps.anl.gov/Users/Meeting/2008/. **Invited talk presented by M. Wood**—Workshop 2: SAXS and SANS Applications in Nano Materials and Nano Biology.
91. J. Burress, M. Wood, S. Barker, J. Pobst, R. Cepel, G. Suppes, P. Shah, P. Buckley, M. Benham, M. Roth, C. Wexler, and P. Pfeifer, "Nanoporous Biocarbon as High-Capacity Storage Material for Hydrogen." In: *International Symposium on Materials Issues in a Hydrogen Economy, Richmond, VA, November 12-15, 2007. Scientific Program and Abstracts Book (Richmond Conference Series, 2007),* p. W-10. http://www.has.vcu.edu/phy/ishe/. **Poster presented by J. Burress and C. Wexler**.

IV - Personnel Working on the Project

Notes: * These are our best estimates for the complete funding periods
* Department affiliations refer to place of work/supervision.
* Percentages reported refer to DOE project; if percentages add up to less than 100%, the individual's research/work obligation for the DOE project is less than 100%. Numbers rounded.

Graduate Students:	
Raina Olsen, Physics:	33% support from DOE (Ph.D, May/2011)
Matt Beckner, Physics:	80% support from DOE (Ph.D., May/2012)
Monika Golebiowska, Physics:	50% support from DOE (M.S, May/2011)
Jimmy Romanos, Physics:	25% support from DOE (Ph.D., May/2012)
Michael Kraus, Physics:	67% support from DOE (Ph.D., Dec/2010)
Elmar Dohnke, Physics:	80% support from DOE
David Stalla. Physics:	80% support from DOE
Matt Connolly, Physics:	70% support from DOE (Ph.D. expected 2014)
Joe Schaeperkoetter, Physics:	100% support from other sources
Tyler Rash, Physics:	100% from other sources (Ph.D. expected 2014)
E. Leimkuehler, Chem. Eng.	100% from other sources
Y.C. Soo, Physics	100% from other sources (Ph.D. expected 2014)
Brian Sawyer, Chem. Eng.	30% support from DOE
Uday Shriniwar, Physics	30% support from DOE
Mikael Wood, Physics:	80% support from DOE
Undergraduate Interns	
Lauren Aston, Physics	25% support from DOE
Sara Carter, Physics	25% support from DOE
Jeffrey Pobst, Physics	25% support from DOE
Daniel Christian Van Hoesen, Physics	25% support from DOE
Visitors:	
Bogdan Kuchta, Physics:	Visiting Professor from University of Marseille, France 8% support from DOE
Lucyna Firlej, Physics:	Visiting Professor from University of Montpellier II, France 8% support from DOE
Postdocs:	
Hanbaek Lee, Radiology:	100% from other sources
Anupam Sing, Chemistry	100% from other sources
Zhi Yang, Radiology	20% support from DOE
Faculty:	
Peter Pfeifer, Physics:	8% support from DOE
Carlos Wexler, Physics:	8% support from DOE
Fred Hawthorne, Radiology:	4% support from DOE
Jacob Burress, Physics:	20% support from DOE
Galen Suppes, Chem. Eng.	100% from other sources
Satish Jalistegi, Radiology:	100% from other sources
Mark Lee, Radiology:	100% from other sources
H. Taub, Physics:	100% from other sources
P. Yu, Physics:	100% from other sources
Jan Ilavsky, Argonne National Lab:	100% from other sources
Technical:	
Ali Tekkei, Chemical Eng.:	100% from other sources