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

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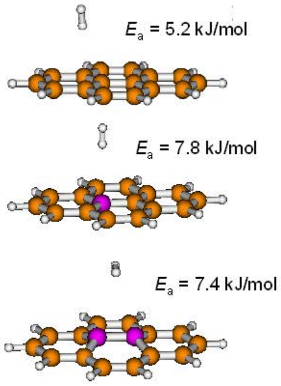
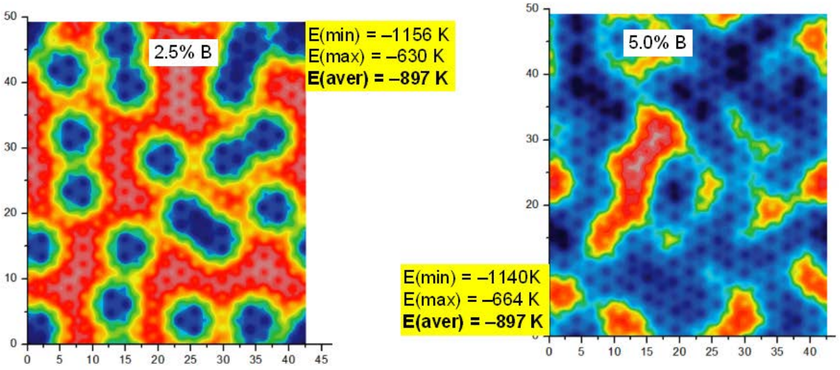
Objectives & Relevance

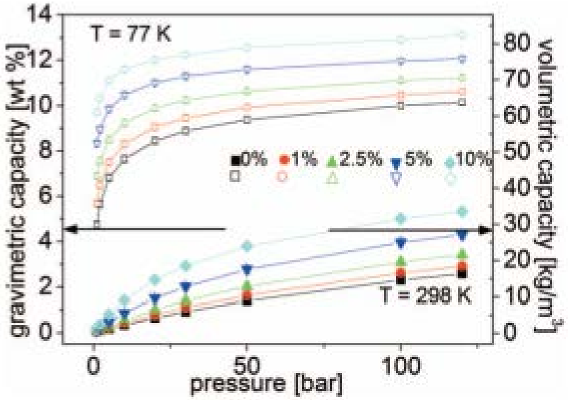
- Synthesize boron-doped and nitrogen-doped pore networks, from polymeric materials, for H_2 storage with high surface areas
  - boron predicted to raise binding energy from 5 kJ/mol to 10-15 kJ/mol
- Characterize materials and mechanisms of H_2 adsorption
  - Structure and thermodynamics of adsorbed adsorbed films from 4K to 300 K (subcritical and supercritical adsorption)
  - Integrated experimental and computational program
  - carbons offer much richer spectrum of high-capacity adsorbents for H_2 than previously appreciated
- Function-driven materials design for hydrogen storage (2017 DOE Hydrogen Storage Targets)

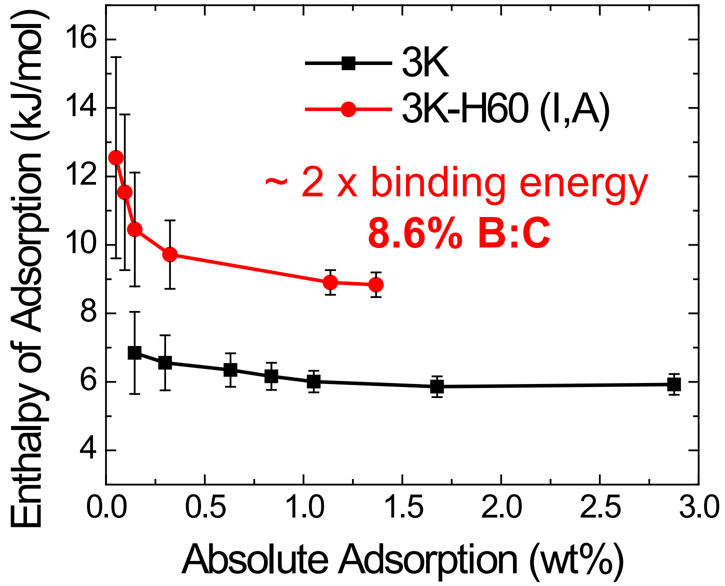
Background

BES (2009): *ab initio* calculations: enhanced adsorption in B-doped carbon









~ 2 x binding energy

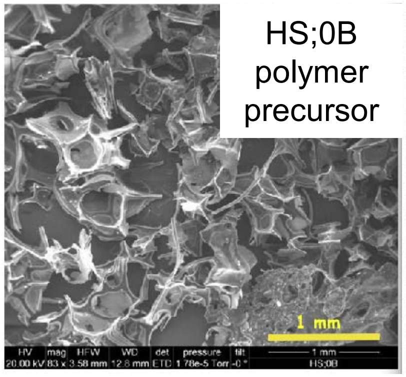
8.6% B:C

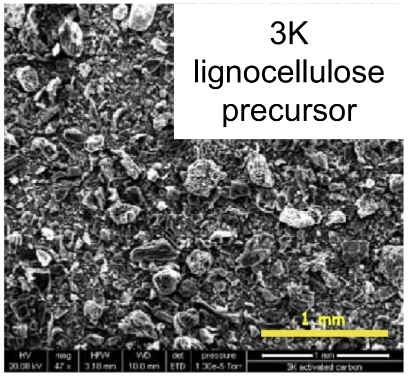
EERE (2012): decaborane doped activated carbon from corncob (**8.6% B:C**), 2000-2500 m^2/g

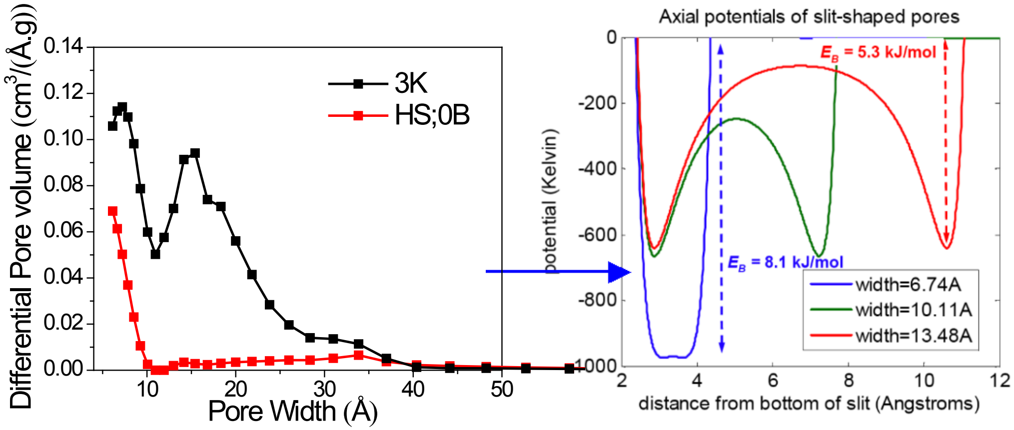
Approach

Why boron-doped carbon via co-polymerization?

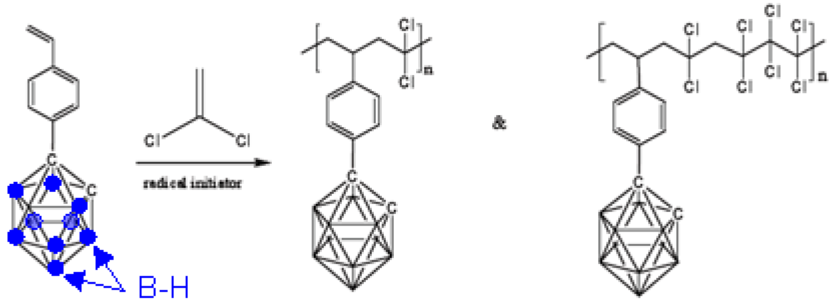
- Monodisperse boron and narrow pores ➔ higher H_2 binding energies

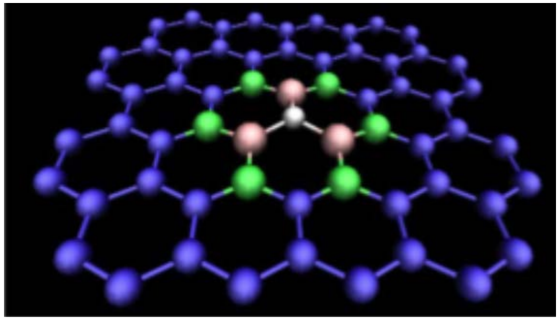

HS;0B polymer precursor


3K lignocellulose precursor



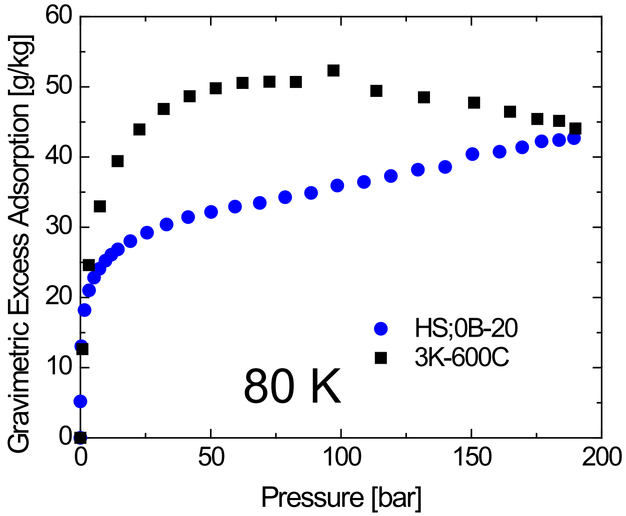
- Easier incorporation of boron into the carbon matrix





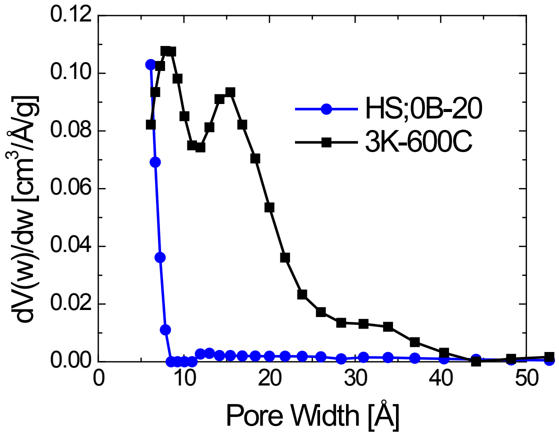
Technical Accomplishments

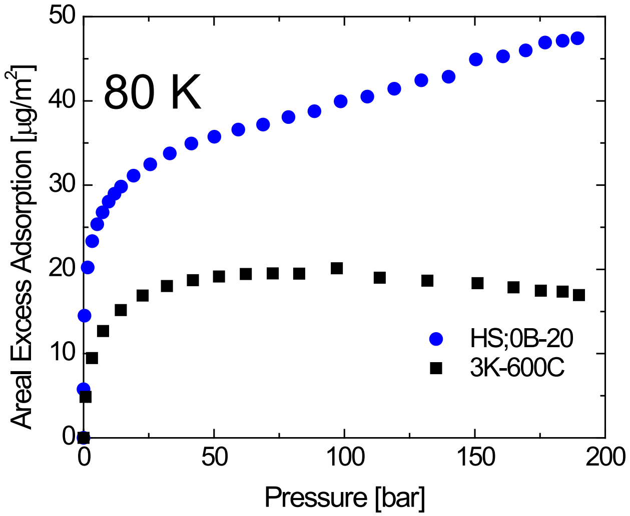
Synthetic Carbon Enhanced Adsorption

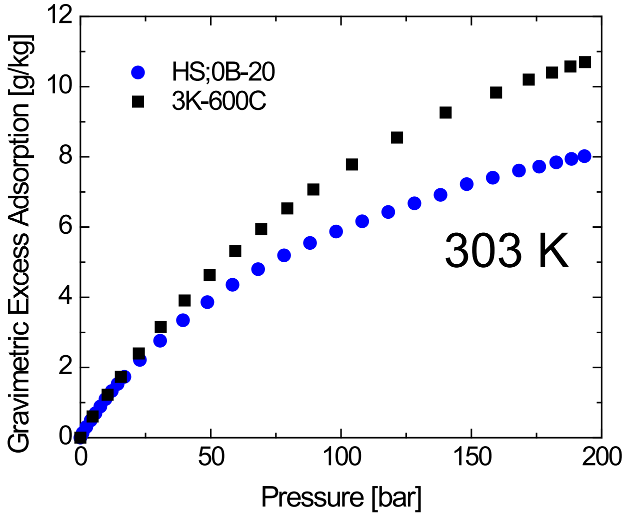


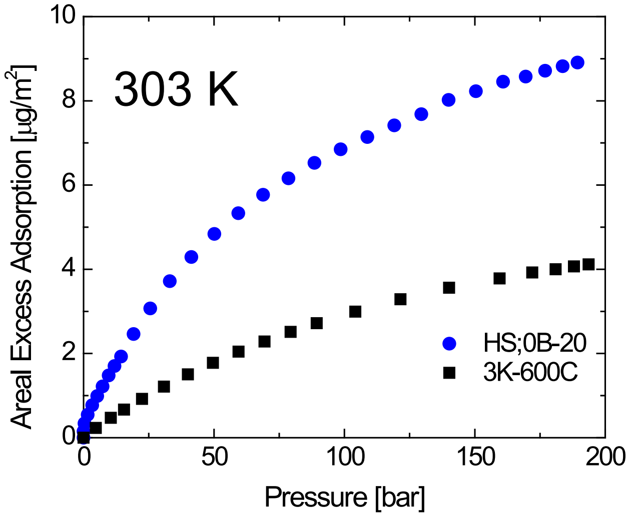
Synthetic carbon, HS:0B, is anomalous:

- Maximum in exc. ads. at higher than normal pressure
- Much higher exc. ads. per unit area than other carbons





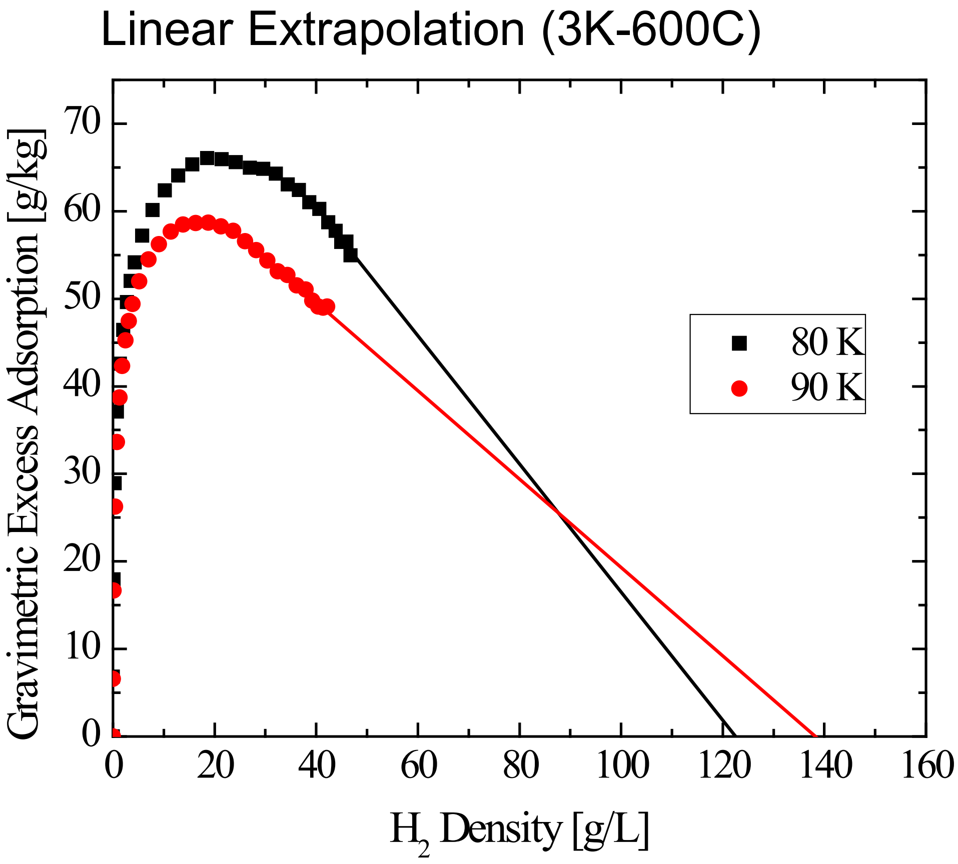




Sample	Surface Area (m^2/g)	Porosity	Areal Excess @ 303K, 100 bar ($\mu g/m^2$)
HS;0B-20 synthetic	900	0.46	6.9
3K-600C lignocellulose	2600	0.76	2.9

Hydrogen Film Density

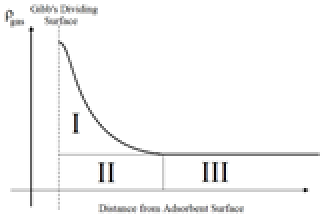
- When adsorbed film density is equal to the bulk gas density the excess adsorption is zero
- *x*-intercept should give approximation of adsorbed film density
- Saturated film density is ~ twice the liquid density
- Synthetic carbons need to be measured at temperatures < 77K to get a strong maximum to perform extrapolation



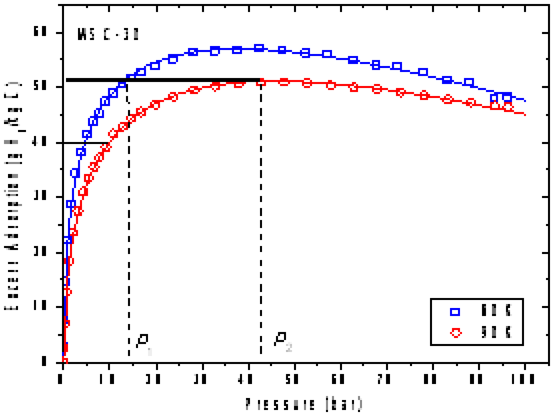
Sample	Saturated Film Density [g/L]
Liquid H_2 (at 20 K)	71
3K-600C (from 80 K)	120
3K-600C (from 90 K)	140

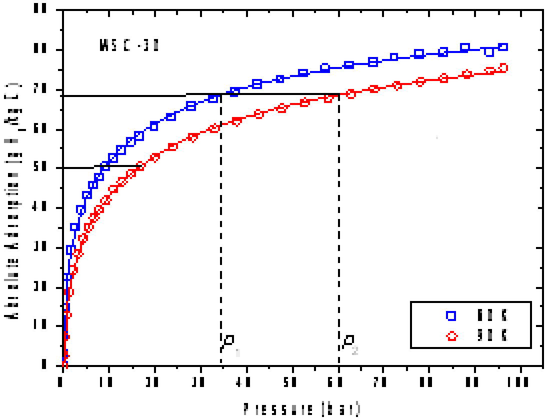
Hydrogen Film Thickness

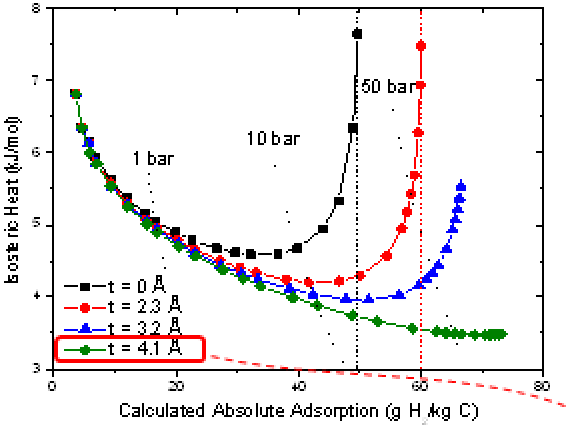
$$\Delta_{ads}H(\theta) = \frac{RT_1T_2}{T_2 - T_1} \ln\left(\frac{p_2(T_2,\theta)}{p_1(T_1,\theta)}\right)$$



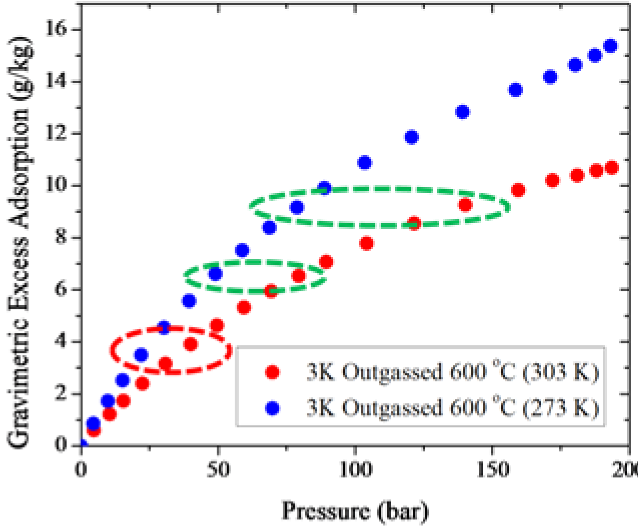
2011: 80-90 K

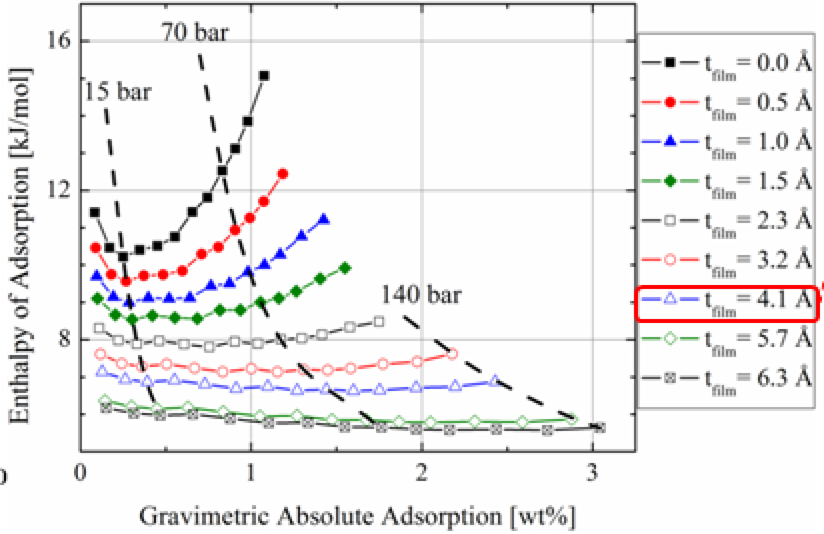






2012: 273-303 K





Film volumes from isosteric heats (this slide) consistent with high-pressure extrapolated film densities (prev. slide)

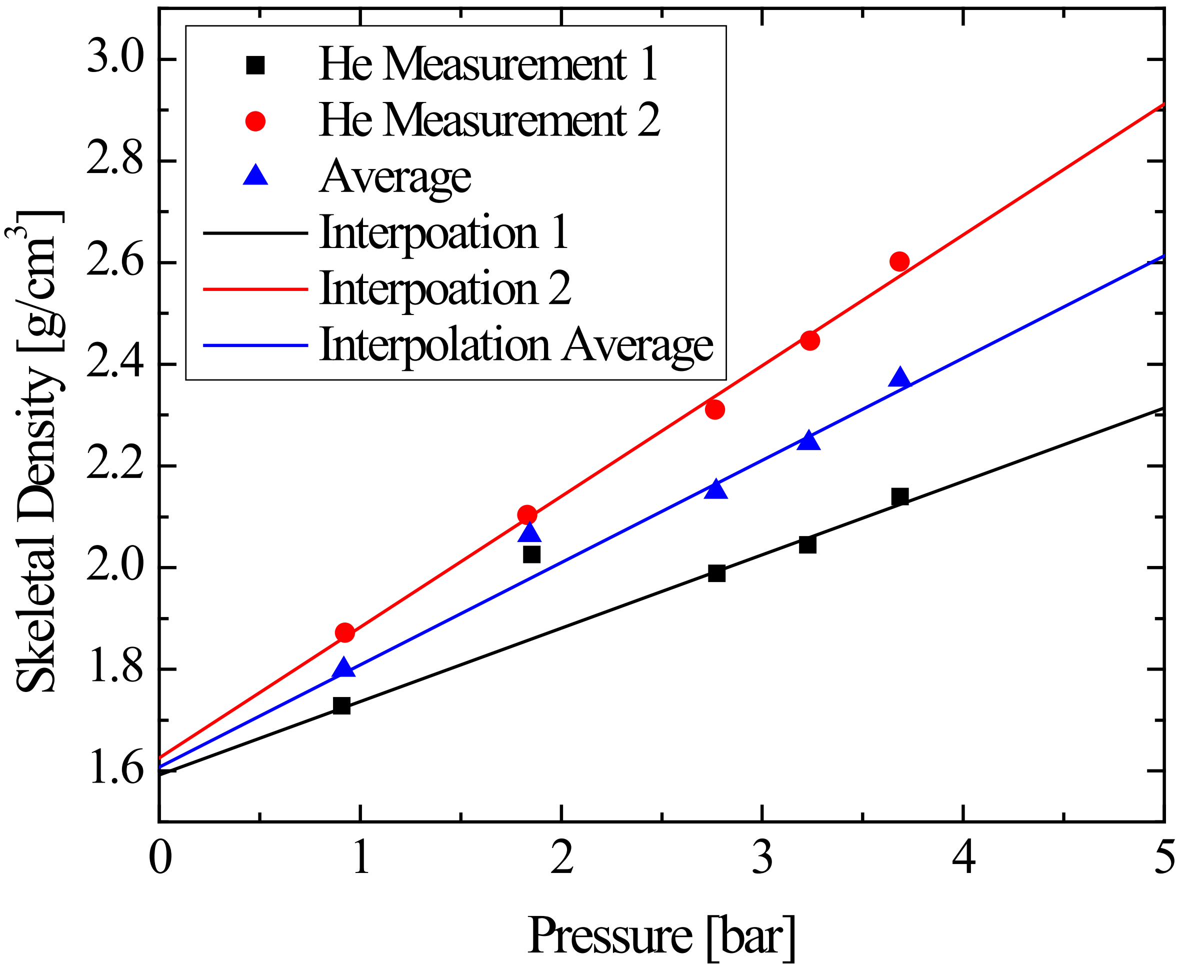
Skeletal Density from Henry's Law Regime

- High surface area carbons adsorb helium even at room temperature
- True skeletal density, ρ_0, determined from Henry's Law
- Extrapolate isotherm to zero pressure where adsorption is negligible

$$\rho_{\text{observed}} = \rho_0 + k_{\text{H},\rho} p$$

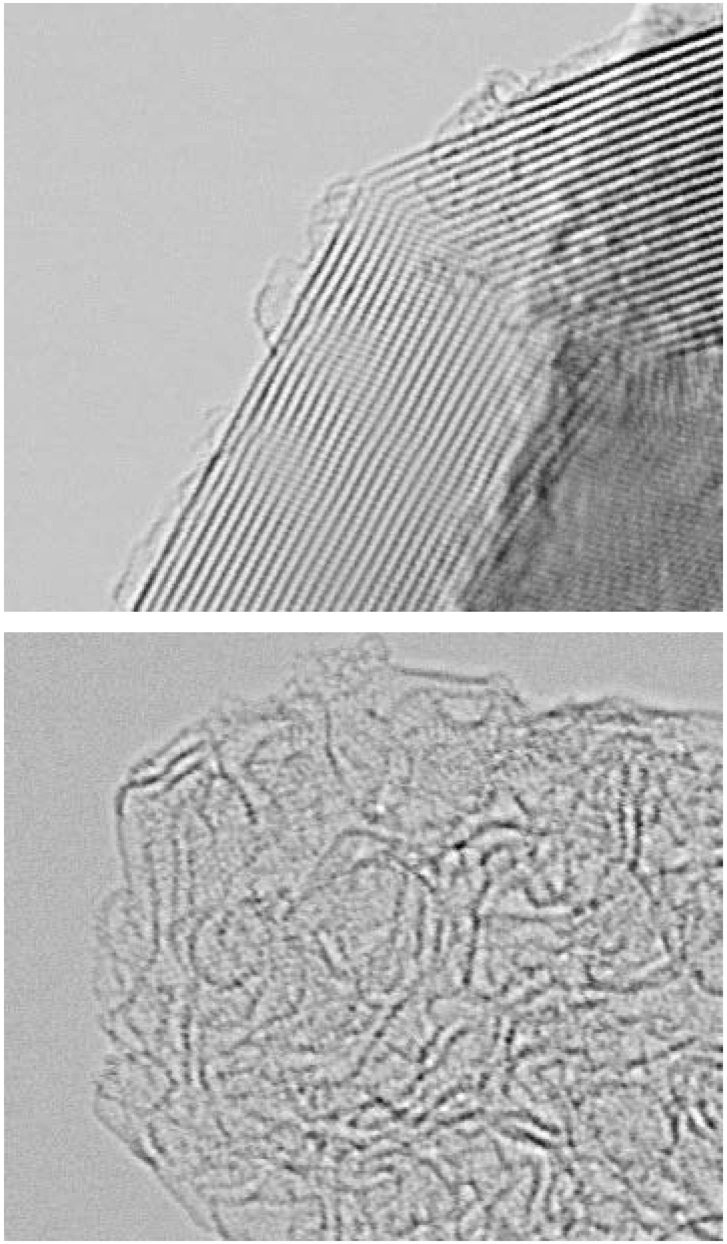
- ρ_0 = 1.6 ± 0.1 g/cm^3
- *When validated, hydrogen storage on numerous carbons will need to be revised upward*

Room Temperature
Helium Isotherm (3K-600C)



High Resolution Transmission Electron Microscopy

- Oak Ridge National Laboratory
  - Center for Nanophase Materials Sciences
- Aberration corrected STEM
  - Nion UltraSTEM with 200 kV cold field emission gun
  - Full 5th order aberration corrector
  - Measured at 60 kV for carbon
- Polymer carbons have regions of graphitic and amorphous carbon consistent with 700 m^2/g surface area

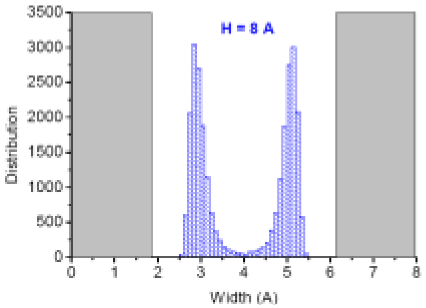


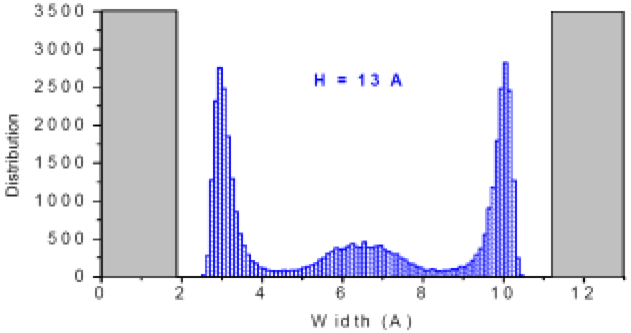
Numerical Modeling (GCMC)

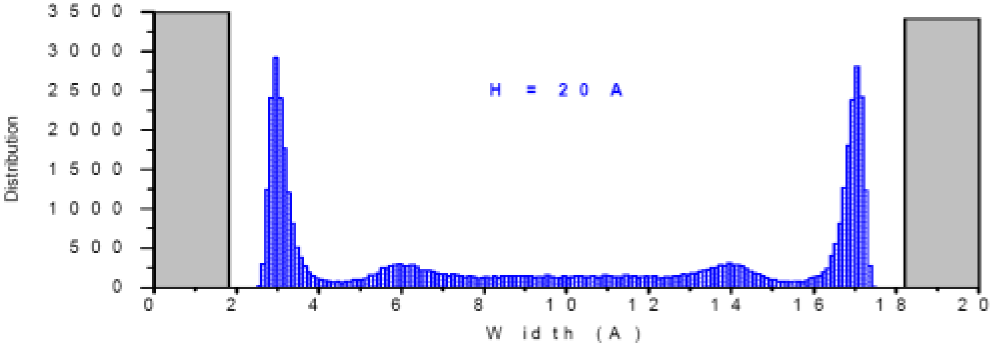
Density distribution for participating pores, with carbon volume represented by grey walls (GCMC)

Experimental pore size distribution from N_2 adsorption at 77 K

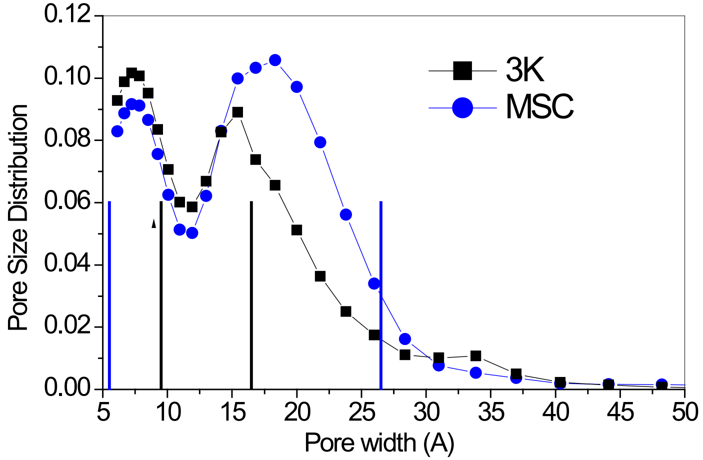
Temperature: 80 K

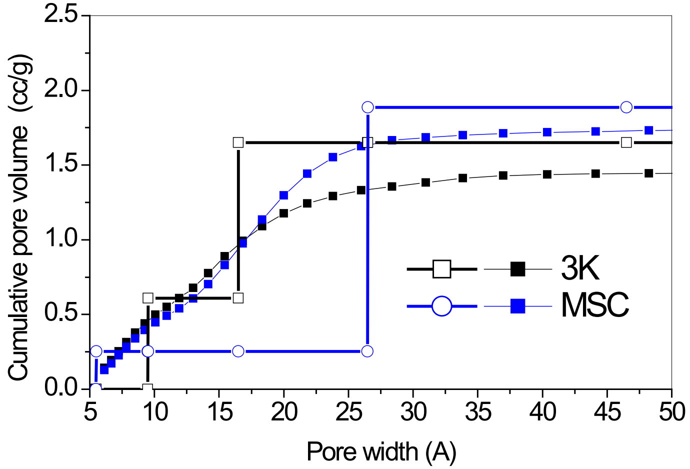






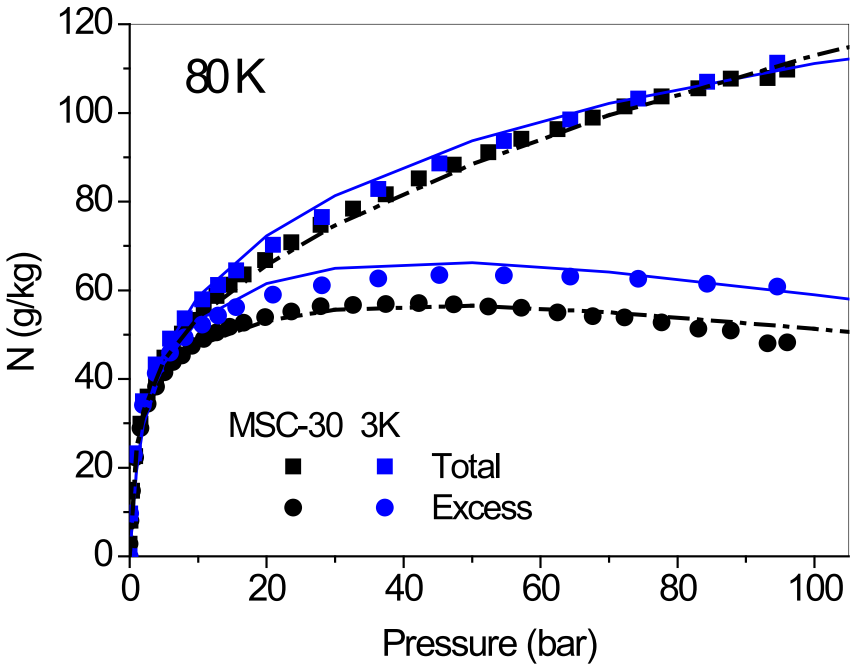
Second layer formation for pores between 10-20 Å

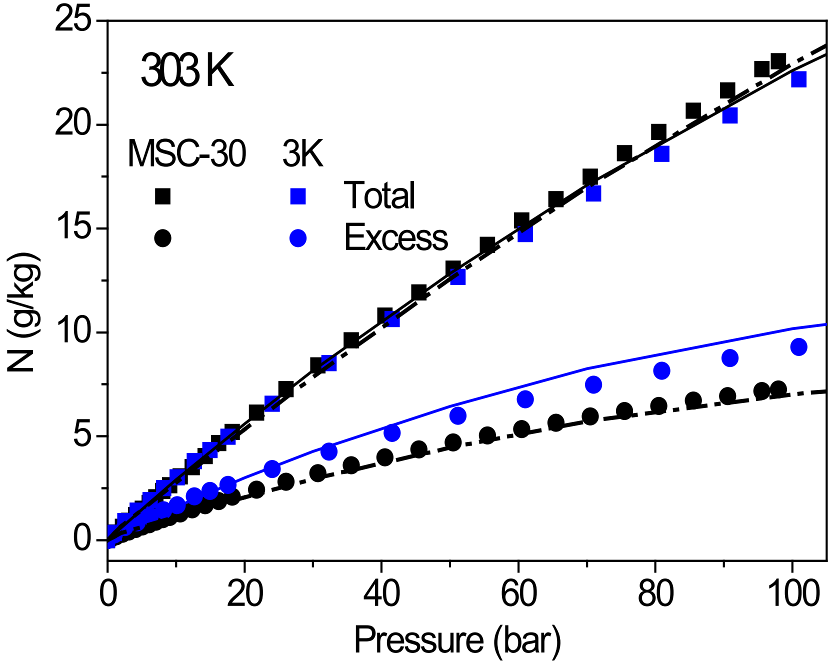




Numerical Modeling (cont.)

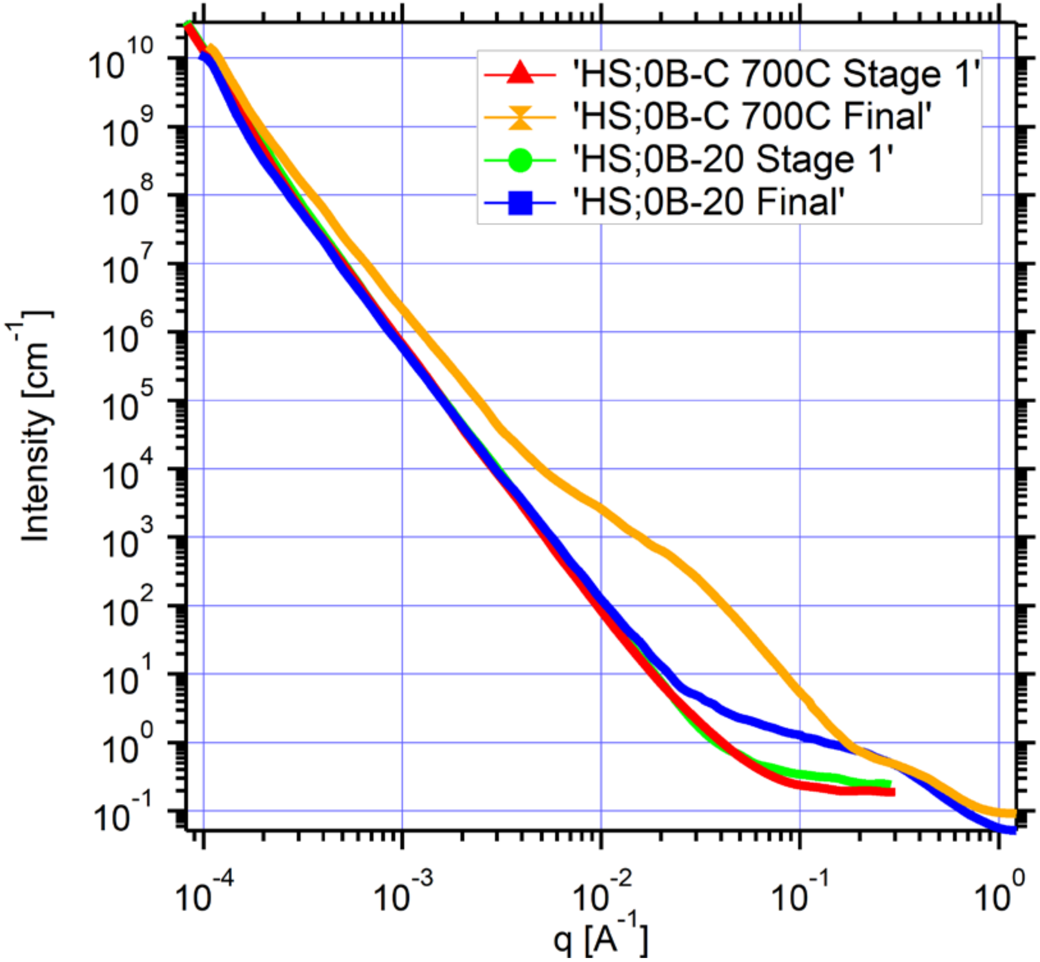
Lines represent the numerical simulation fits:
3K: 50% H13 + 50% H20 (Hxx: slit pore of width xx Å)
MSC-30: 50% H8 + 50% H30





Bimodal model correctly predicts:
- Grav. excess adsorption
- Grav. storage capacity
- Isotherms at 80 K
- Isotherms at 303 K

Small Angle X-ray Scattering of Synthetic Carbon



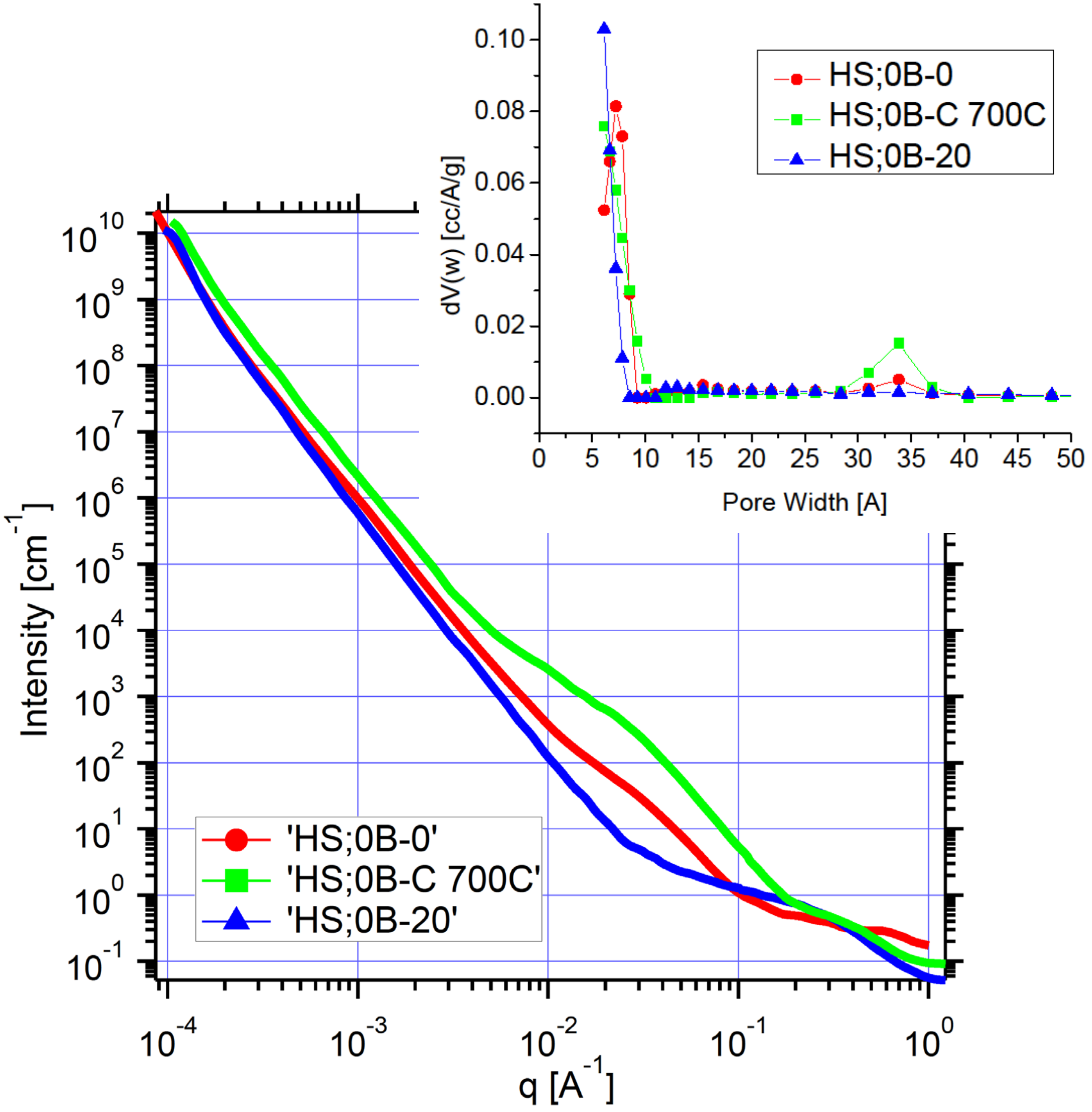
Stage 1: initial pyrolysis to ~250 C
Final: pyrolysis finished to 700-1000 C

- It is shown that the first stage of heating (outgassing) has little effect on the ultimate structure, with characteristic pores forming during the second stage (pyrolysis)
- For q<~3x10^{-3} Å^{-1}, all graphs share a common power law of approximately q$^{-3.6}$, indicative of a surface fractal network with D_s = 2.4
- To study the effect on the nanopores, the data at q>0.3 Å^{-1} is modeled using a Guinier fit to determine the radius of gyration :

$$I(q) = G\ \exp\left[\frac{(q\,R_g)^2}{3}\right]$$

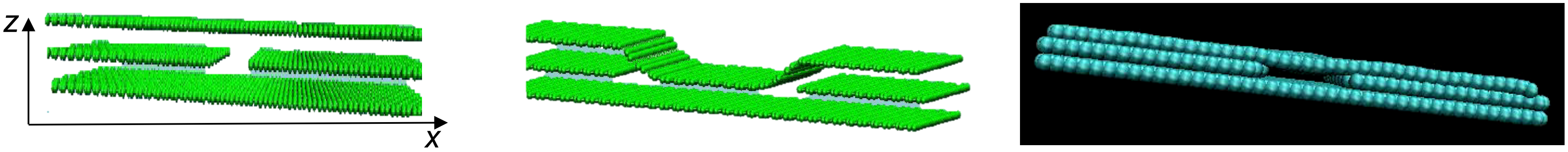
Small Angle X-ray Scattering

Model	**HS;0B-0**	**HS;0B-C Large**	**HS;0B-C Small**	**HS;0B-20**
Radius of Gyration	60 Å	70 Å	3 Å	5 Å
Sphere Diameter	140 Å	170 Å	9 Å	12 Å
Circle Diameter	160 Å	190 Å	9 Å	13 Å
Square Side Length	140 Å	160 Å	8 Å	11 Å
Triangle Side Length	190 Å	230 Å	12 Å	16 Å
Ave Pore Width (SAXS, knee)	180 Å	190 Å	16 Å	21 Å
Ave Pore Width (N_2 Sorption)	19 Å	20 Å		18 Å



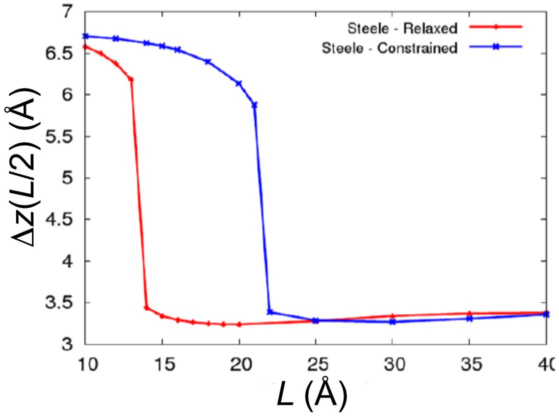
Conformability of Pores

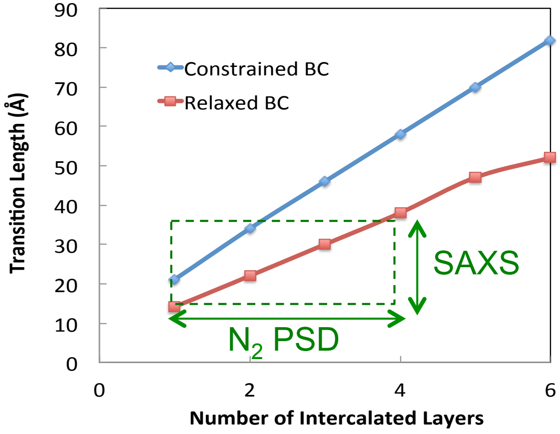
- Is there a maximum lateral size for a slit pore?
- Will pores “collapse” if they are too large?
- Does this depend on the presence of adsorbed gas?
- Is there a pressure-dependent pore volume?



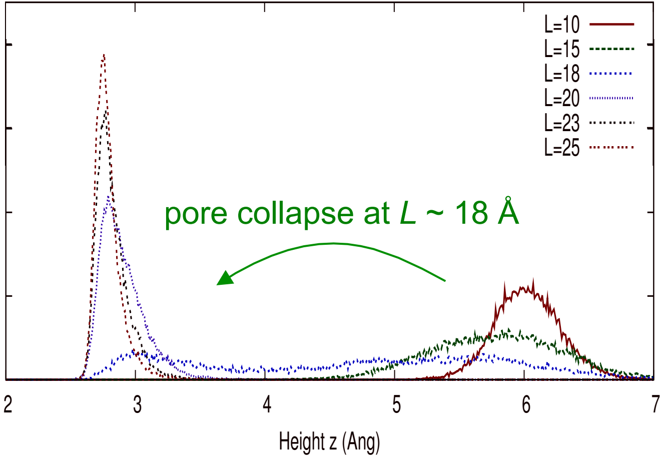
Minimize: $$E[z(x)] = \int [\underbrace{2C(\nabla^2 z)^2 + V_{\text{attr.}}(z)}_{\Gamma(z)}]\,dx \Rightarrow \frac{\partial\Gamma}{\partial z} - \frac{d}{dx}\left(\frac{\partial\Gamma}{\partial z'}\right) + \frac{d^2}{dx^2}\left(\frac{\partial\Gamma}{\partial z''}\right) = 0$$

Center Opening vs. Pore Length





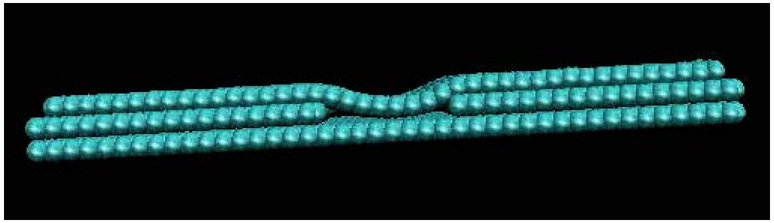
Pore center opening distribution



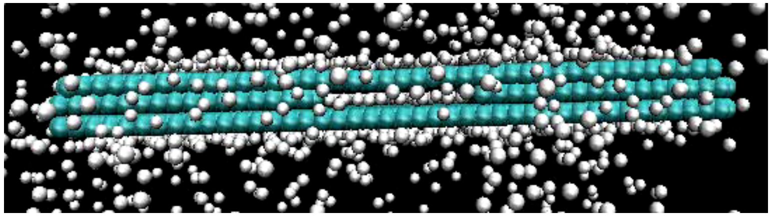
Conformability of Pores

- Is there a maximum lateral size for a slit pore?
- Will pores “collapse” if they are too large?
- Does this depend on the presence of adsorbed gas?
- Is there a pressure-dependent pore volume?

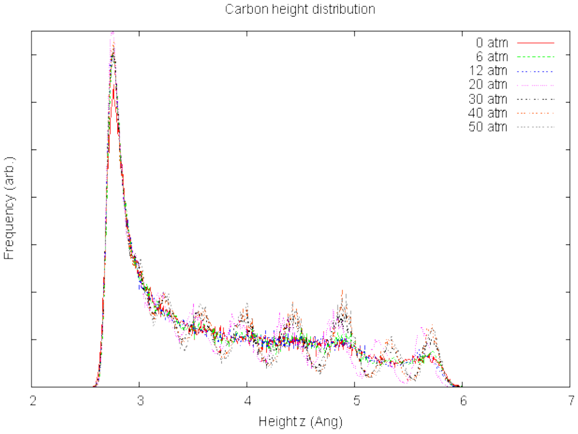
L = 20 Å, no gas ➔ collapsed pore



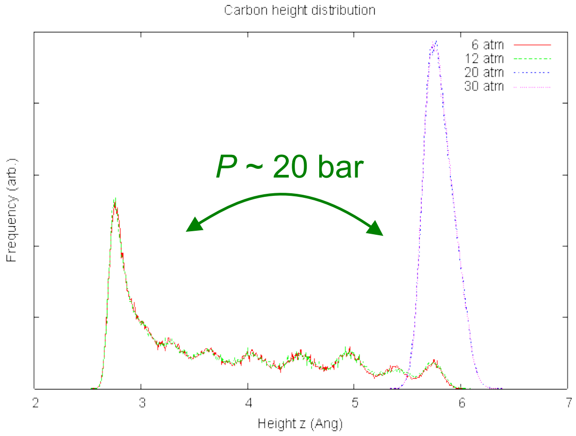
L = 25 Å @ 30 bar



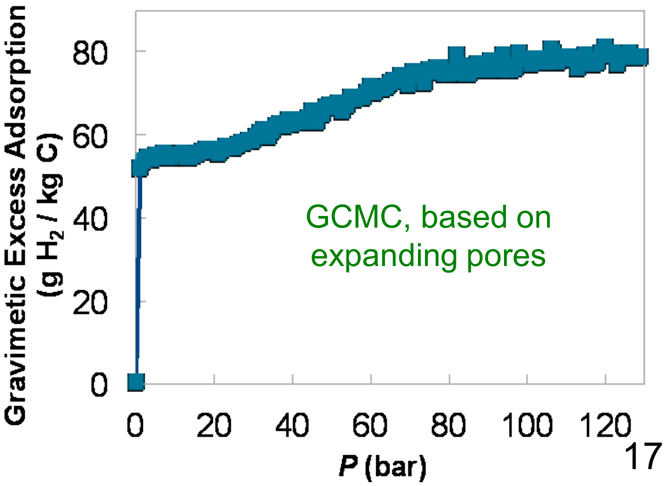
L = 25 Å, collapsed pore being filled (~ 1μs, 10^6 steps)



(pre-filled) Open/close “transition” at ~ 20 bar

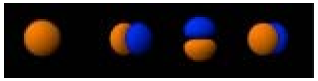


Expanding Slit-Shaped Carbon Pore



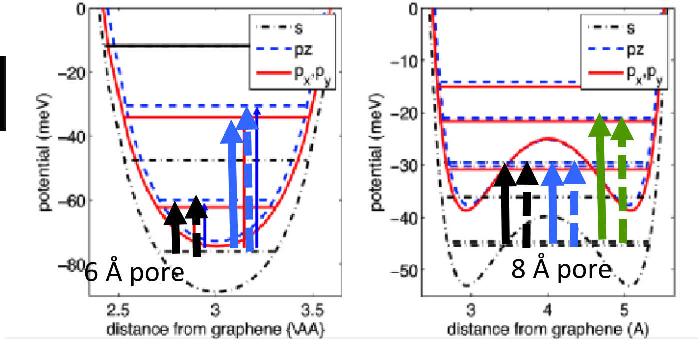
Incoherent Inelastic Neutron Scattering

Theory: sub-nm characterization of pores (2011)



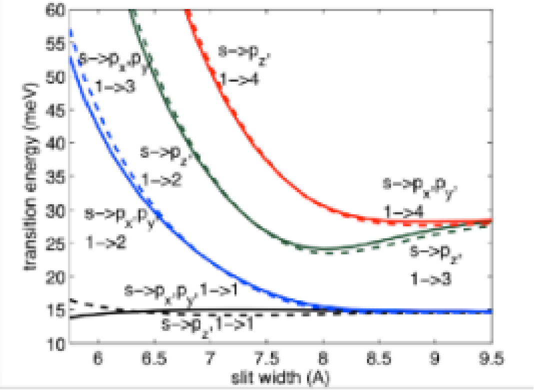
$$E_J = J(J+1)\frac{\hbar^2}{2\mu r^2},$$

$E_1 - E_0 = 14.7$ meV

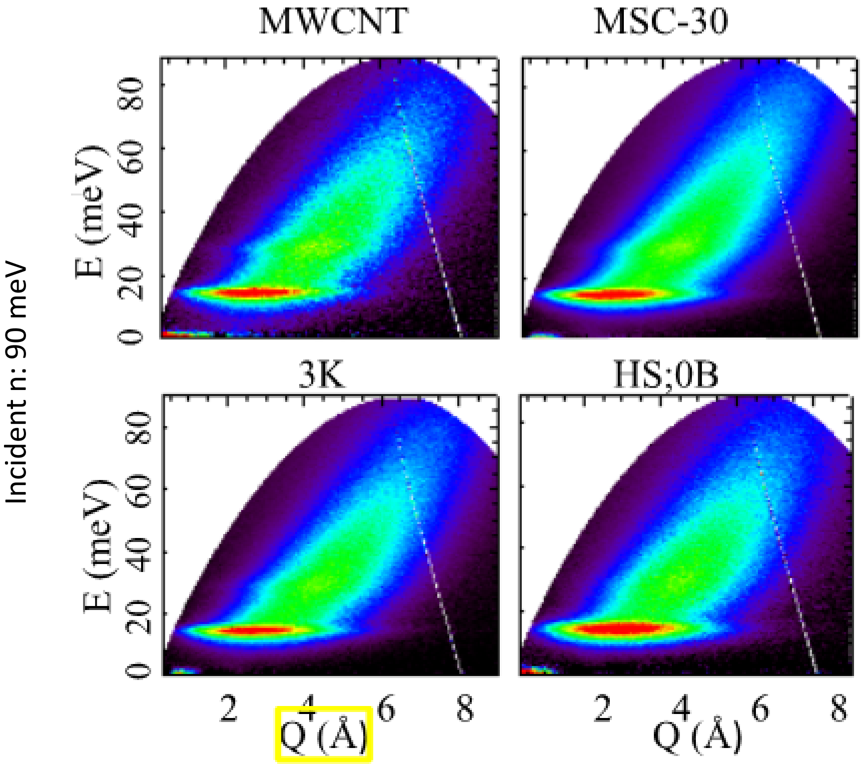


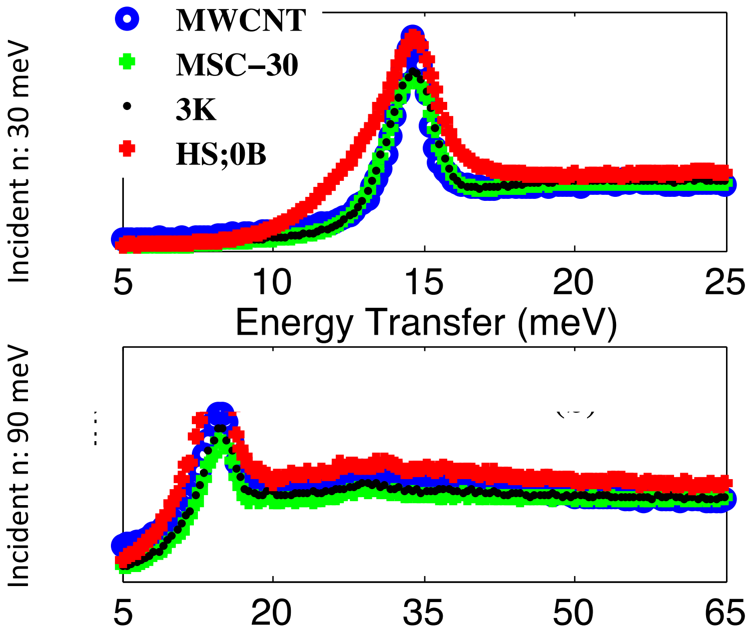
← Quantum levels for adsorbed H_2

IINS peaks vs. pore width →



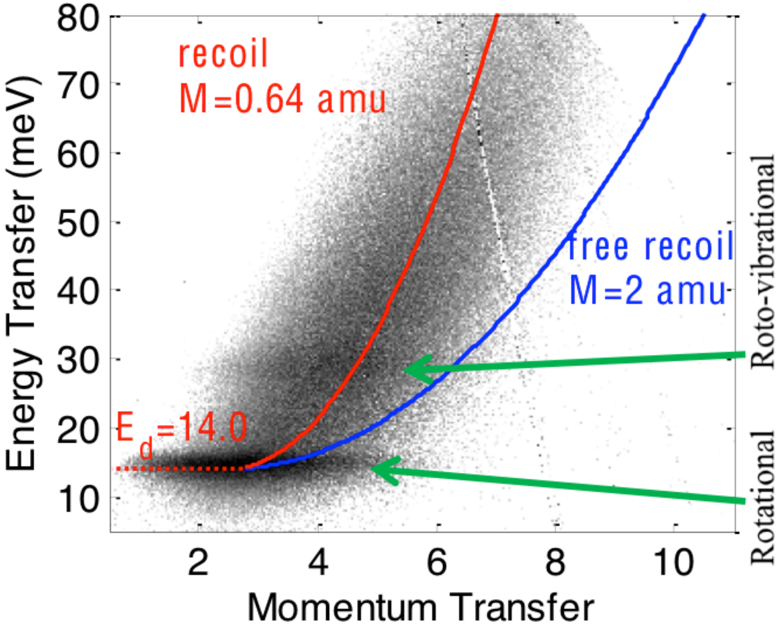
Experiment at ORNL (2012)





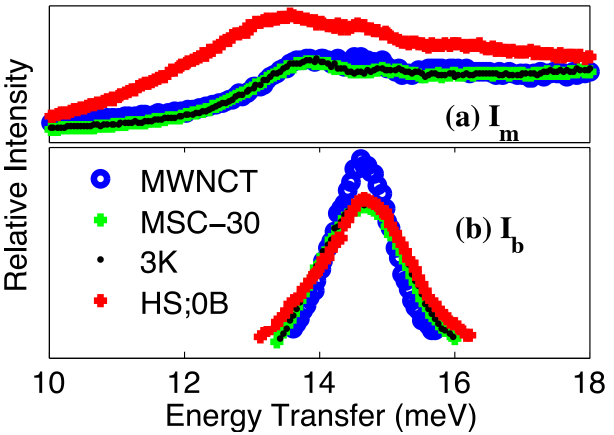
Incoherent Inelastic Neutron Spectroscopy

Decomposition into *mobile* and *bound* adsorbed H_2 states (2011-12)



$$S_m(Q,E) = (a + b\Delta E)F_{||}(Q - Q_R)e^{-exp(c\Delta E)dQ^2}$$

$$S_b(Q,E) = fe^{(E-E_b)^2/2g^2}F_{\perp}(Q)e^{-hQ^2}$$



Interpretation:

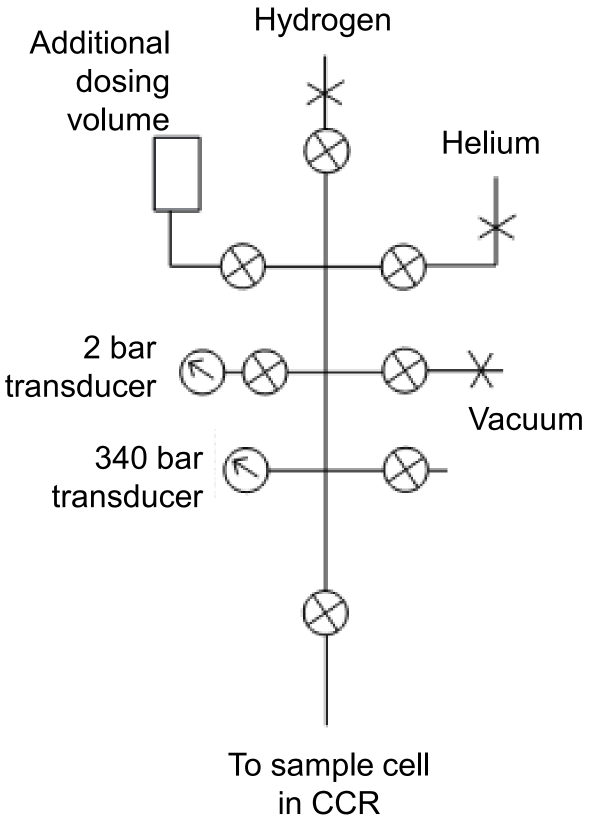
Similarities of spectra for samples with very different PSDs suggest* very few sub-nm pores in AC, most pores with similar binding energies. *Except HS;0B

Two types of states: mobile & bound, different adsorption properties? (Burress *et al., Nanotechnology* 2009)

Different weights of S_m and S_b in different samples indicate (small) differences in the degree of "planarity" of the substrate on a supra-nm scale. The area of S_m peak for the ACs is ~ 95% of that of the MWCNTs (a nominally smooth surface), and the area of S_b is 105% for ACs vs. MWCNTs, while significantly wider. Interpretation: AC's are almost as smooth as MWCNTs (at 1-2 nm lengths).

Sievert Apparatus

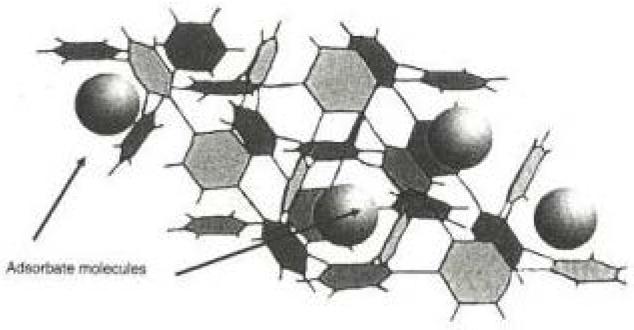
- Pressure range
  - 0-200 bar
- Temperature range
  - 8-500 K using closed cycle refrigerator
- Temperature stability
  - ±0.01 K
- Sample size: 0.5-2 g
- Gases: helium, hydrogen, methane, mixtures, etc…
- Allow hydrogen BET measurements using subcritical hydrogen



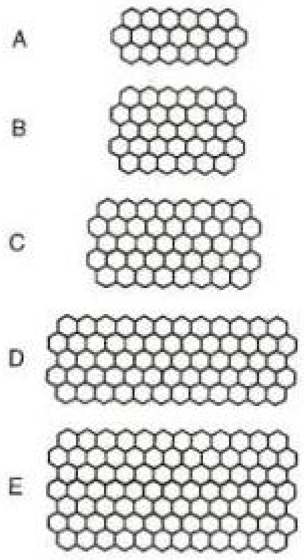
⊗ Pneumatic controlled valve

X Needle valve

Geometrically Optimized Models for Adsorption



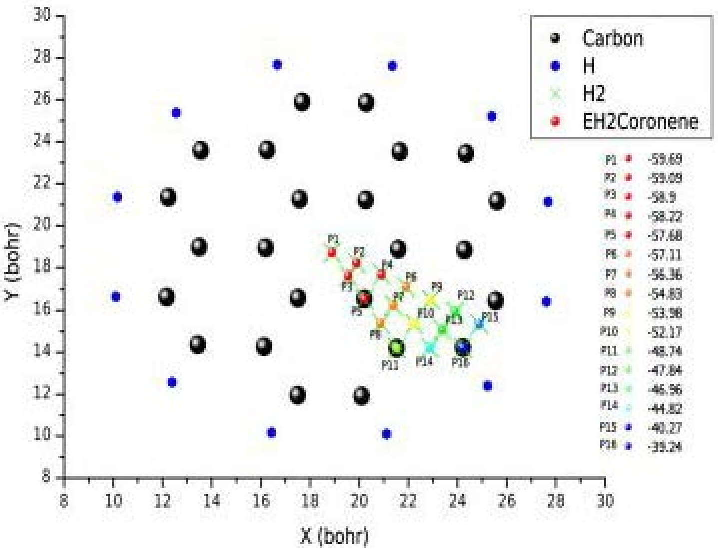
Polyphenylene model based on concepts of Gibson et al. (1946) and Riley (1947)



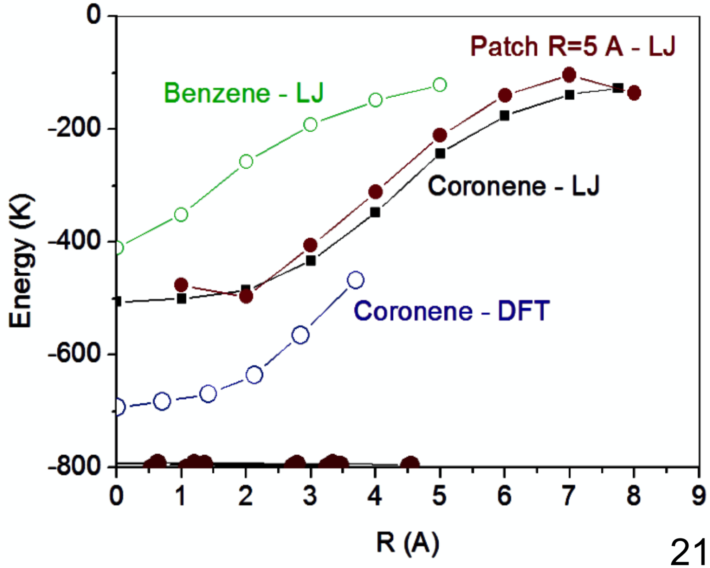
The model of Kaneko (1992)

Mol	# of C	size(nm)	Surface (m^{2}g^{-1})
A	56	1.1x2.1	5800
B	71	1.5x2.1	6000
C	110	1.5x2.6	4700
D	158	1.5x3.5	4400
E	212	1.9x3.5	4100

Model: adsorption on “circular” fragments

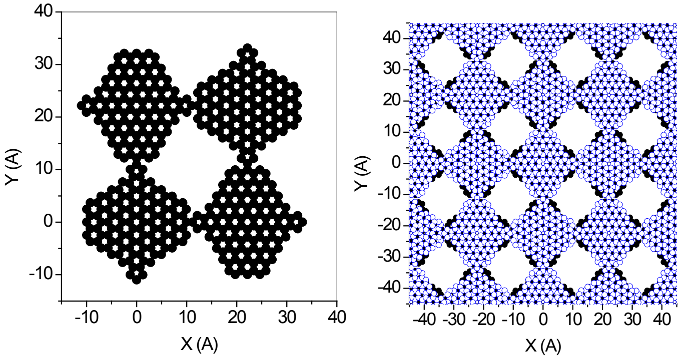


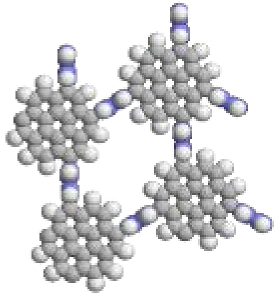
Competition between increasing surface and weaker binding energy



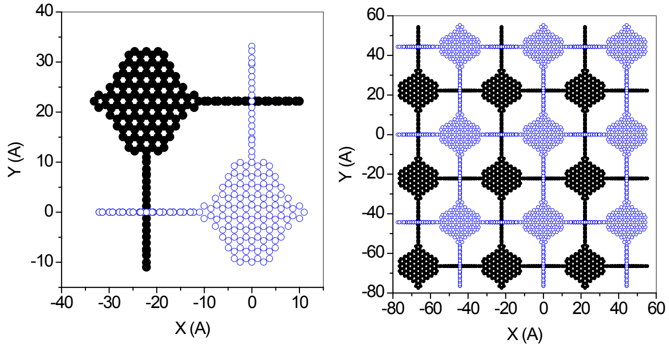
Open Carbon Frameworks (GCMC)

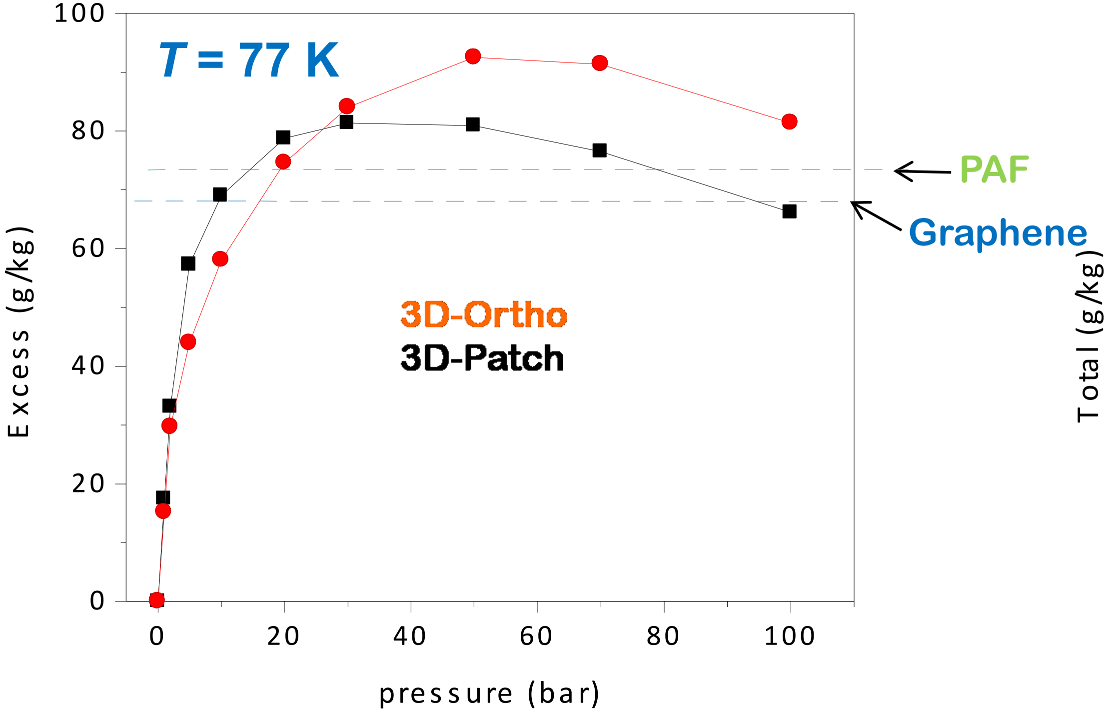
3D-Patch

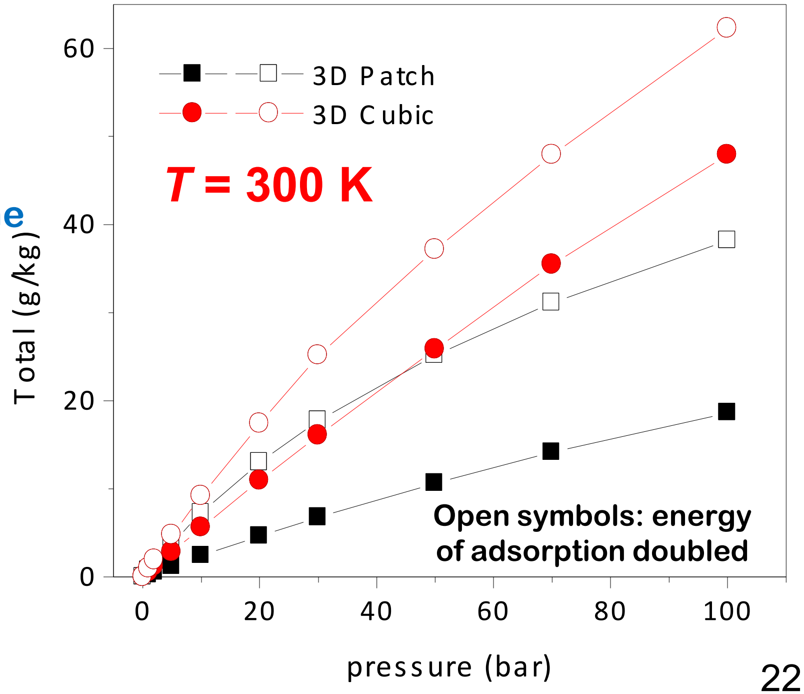




3D-Ortho





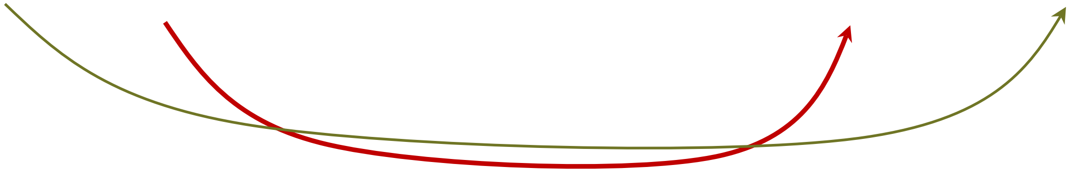


Open symbols: energy of adsorption doubled

Open Carbon Frameworks (GCMC)

Performance Comparison: PAF, graphene, OCF’s, Coronene/Benzene

	PAF-302	PAF-303		3D-Patch	3D-Ortho	Cor_Benz
Surface (m^2/g):	**7100**	**……**	**2600**	**3500**	**4200**	**6500**
Adsorption (g H_2/kg) :						
T = 77 K :	**115**	**170**	**95**	**120**	**265**	**131**
T = 298 K :	**25**	**40**	**20**	**17**	**48**	**25**
Energy of Adsorption:	**<4.6 kJ/mol**		**4.5 kJ/mol**	**<4.5 kJ/mol**	**<4.5 kJ/mol**	
Density (g/cm^3):	**0.32**	**0.16**	**0.76**	**0.48**	**0.16**	**0.40**



Project Summary, 2011-12

- Polymeric carbon enhanced adsorption
  - PVDC carbons show enhanced hydrogen sorption compared to lignocellulose-precursor carbon due to dominance of nanopores
- Hydrogen film density & thickness
  - Hydrogen film density determined from extrapolation of high pressure hydrogen sorption measurements is ~ twice that of liquid hydrogen
  - Elimination of unphysical rise in isosteric heat gives an lower bound to the film thickness
- HRTEM
  - Synthetic carbons have regions of graphite and amorphous carbon
- Small angle X-ray scattering
  - Two shoulders in scattering lead to a large and small structure, the small structure is likely pores whereas the large structure is likely regions of graphite as seen in HRTEM
- Conformability of pores
  - The graphene layers may flex and move with increased pressure
- Incoherent inelastic neutron spectroscopy
  - Two dominant states emerge, mobile and bound
- Open carbon frameworks
  - New theoretical structures will give insight into new materials to be synthesized and the effect of surface area and biding energy in predominantly carbon systems

Future Work: Plans for 2012/13

- Polymeric carbons
  - New copolymerization routes utilizing poly(vinylidene chloride) or poly(vinyl alcohol) with boronic acids or vinyl carboranes
- Neutrons
  - IINS further investigate hydrogen interactions with boron containing substrate at different temperatures and coverages
- Aberration corrected STEM
  - Explain interesting behavior of polymer-based pure carbons
  - Identify position of boron atoms with EELS
- Sieverts
  - Perform low temperature studies of b-doped carbons both at subcritical (hydrogen BET) and supercritical conditions
- Hydrogen measurements
  - Higher pressure measurements on higher binding energy materials to better determine hydrogen film density
  - Study Henry’s law regime to experimentally determine binding energies and vibrational frequencies of hydrogen in b-doped systems
- Simulations
  - GCMC of different optimized structures
  - Conformable pores

Supplemental Slides

Publications

In Progress:

- *The Quantum Excitation Spectrum of Adsorbed Hydrogen*, R. Olsen, M. Beckner, P. Pfeifer, **C. Wexler**, and H. Taub, Phys. Rev. Lett. (under review).
- *Functional B-C Bonds in Nanoporous Boron Carbide and Boron Doped Carbon Materials*, 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 (under review).
- *Elastic Pore Structure of Activated Carbon*, M.J. Connolly and C. Wexler, Phys. Rev. B.
- *Boron Doping of Activated Carbons Using Decaborane*, M.J. Connolly, M.W. Beckner, and C. Wexler, Langmuir.
- *Infrared Study of Boron-Carbon Chemical Bonds in Boron Doped Activated Carbon,* J. Romanos, M. Beckner , D. Stalla, A. Tekeei, G. Suppes, S. Jalisatgi, M. Lee, F. Hawthorne, J. D. Robertson, L. Firlej, B. Kuchta, C. Wexler, P. Yu, and P. Pfeifer.

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- *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).

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- *Numerical Estimation of Hydrogen Storage Limits in Carbon Based Nanospaces*, B. Kuchta, L. Firlej, P. Pfeifer, & C. Wexler, Carbon **48**, 223-231 (2010).
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- *Numerical Analysis of Hydrogen Storage in Carbon Nanopores*, C. Wexler, R. Olsen, P. Pfeifer, B. Kuchta, L. Firlej, Sz. Roszak, Int. J. Mod. Phys. B **24**, 5152-5162 (2010).
- *Multiply Surface-Functionalized Nanoporous Carbon for Vehicular Hydrogen Storage*, P. Pfeifer, C. Wexler, G. Suppes, F. Hawthorne, S. Jalisatgi, M. Lee, & D. Robertson, DOE Hydrogen Program 2010 Annual Progress Report, http://www.hydrogen.energy.gov/annual_progress10. html, p. 474-480.
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- *Hydrogen Storage in Engineered Carbon Nanospaces*; J. Burress, M. Kraus, M. Beckner, R. Cepel, G. Suppes, C. Wexler, & P. Pfeifer; Nanotechnology **20**, 204026 (2009). Featured in http://www.physorg.com/news162195986.html

- *Boron Substituted Graphene: Energy Landscape for Hydrogen Adsorption*; L. Firlej, B. Kuchta, C. Wexler, & P. Pfeifer; Adsorption **15**, 312 (2009).

- *Gas Sorption in Engineered Carbon Nanospaces*, J. Burress, Ph.D. Thesis (University of Missouri, 2009).

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- *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-May, 2012.
- *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-May, 2012.
- *Boron Doping Carbon Structures Using Decaborane: A Theoretical Study*, C. Wexler, M. Connolly, M. Beckner, and P. Pfeifer, *March 2012 Meeting of the American Physical Society* (*Bull. Am. Phys. Soc.* **57**, W33.01 (2012)), Boston, MA, March 2012.
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- *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.

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- *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.
- *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.
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- *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.

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- *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.
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- *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.
- *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.
- *Characterization of activated carbon atsub-nm scale via adsorption (H_2, N_2, CH_4, isosteric heats), TEM, FT-IR, neutron (IINS) & x-ray (SAXS/USAXS); & application towards optimization of H2 storage*, C. Wexler, P. Pfeifer, M. Kraus, M. Beckner, J. Romanos, D. Stalla, T. Rash, H. Taub, P. Yu, R. Olsen, & J. Ilavsky, 9th International Symposium onCharacterisation of Porous Solids (COPS 9), DECHEMA (Gesellschaft für Chemische Technik und Biotechnologie e.V.), Dresden, Germany, June 2011.
- *Inelastic neutron scattering from adsorbed hydrogen*, R. Olsen, M. Beckner, C. Wexler, H. Taub & P. Pfeifer, Wilhelm & Else Heraeus Seminar: Energy Materials Research by Neutrons & Synchrotron Radiation, Bad Honnef, Germany, May 2011.

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- *Nanopore structure from small angle & 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, & P. Pfeifer, Wilhelm & Else Heraeus Seminar: Energy Materials Research by Neutrons & Synchrotron Radiation, Bad Honnef, Germany, May 2011.

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- *Inelastic Neutron Scattering from Hydrogen Adsorbed in Carbon*, R. Olsen, M. Beckner, P. Pfeifer, & C. Wexler, March 2011 Meeting ofAmerican Physical Society (Bull. Am. Phys. Soc. 56, H20.11 (2011)), Dallas, TX, March 2011.

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- *Inelastic Neutron Scattering from Adsorbed Hydrogen*, R. Olsen, M. Beckner, H. Taub, & C. Wexler, Fall 2010 Meeting of Prairie Section of American Physical Society, Chicago, IL, November 2010.
- *A Brief History of Energy*, C. Wexler, Global Issues Colloquium (Public Lecture), C. Wexler Truman State University, Kirksville, MO, September 2010.
- *Adsorption of Hydrogen in Boron Substituted Carbon-Based Porous Materials*, L. Firlej, B. Kuchta, P. Pfeifer, & C. Wexler, 10th International Conference on Fundamentals of Adsorption (FOA10), Awaji, Hyogo, Japan, May 2010.
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- *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, & P. Pfeifer, March 2010 Meeting of American Physical Society (Bull. Am. Phys. Soc. 55, T30.07 (2010)), Portland, OR, March 2010.
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- *Natural Gas & Hydrogen Storage for Advanced Transportation*, P. Pfeifer, invited presentation, MU Research & Development Advisory Board, University of Missouri, Columbia, November 2009.
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- *Hydrogen Adsorption in Boron Doped Nanoporous Carbon*, C. Wexler, P. Pfeifer, Sz. Roszak, B. Kuchta, & L. Firlej, 33rd International Workshop in Condensed Matter Theories (CMT33), Ecuador, August 2009.

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- *Hydrogen Storage in Engineered Carbon Nanospaces: Experimental Results & Theoretical/Computional Analysis*, C. Wexler, J. Burress, R. Cepel, B. Kuchta, L. Firlej, & P. Pfeifer, Seventh International Symposium Effects of Surface Heterogeneity in Adsorption & Catalysis on Solids (ISSHAC-7), Poland, July 2009.
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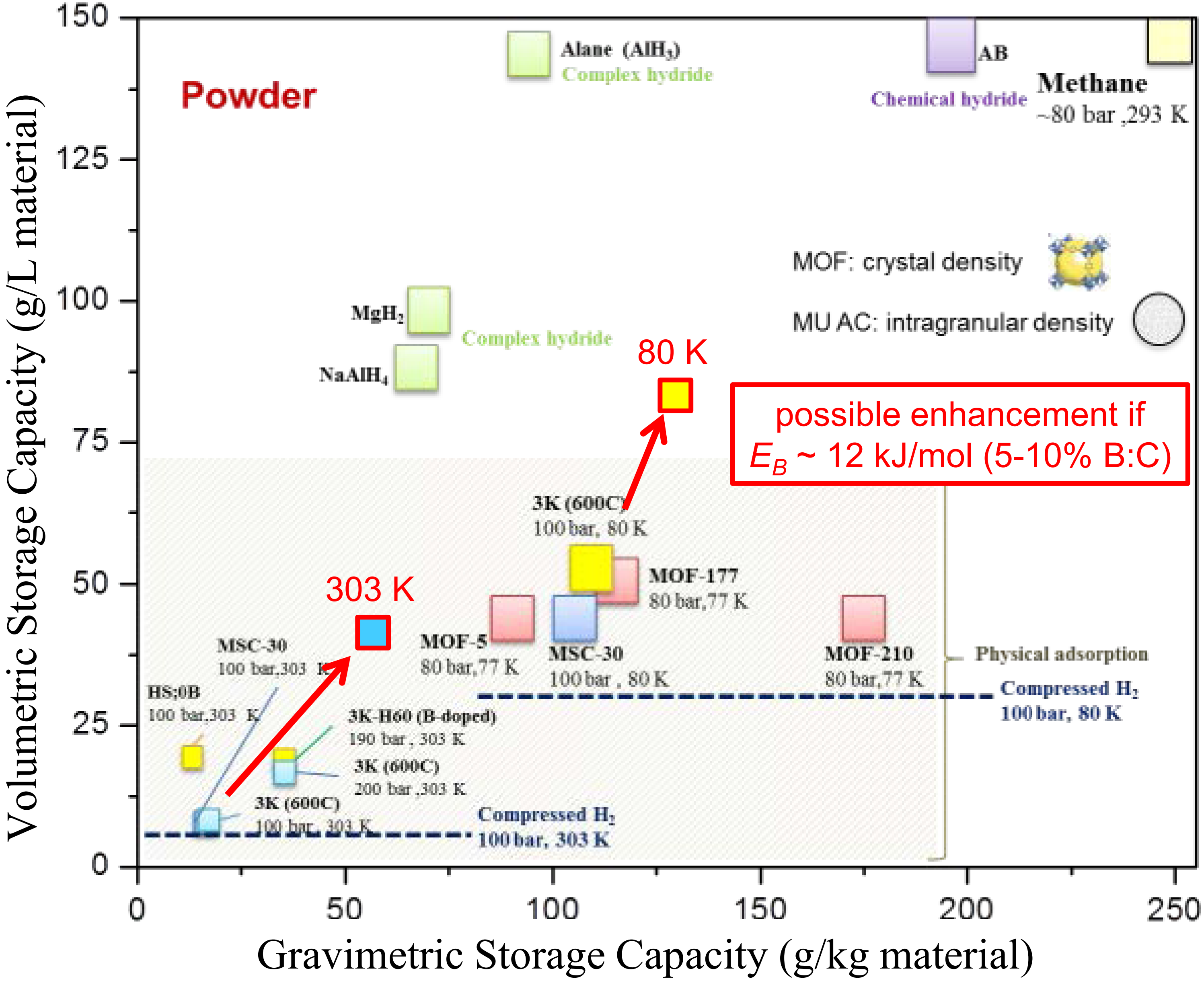
Presentations

- *Structural & Energetic Factors in Designing a Perfect Nanoporous Sorbent for Hydrogen Storage*, B. Kuchta, L. Firlej, R. Cepel, P. Pfeifer, & C. Wexler, 2009 March Meeting of American Physical Society, Pitts-burgh, PA, March 16-20, 2009. Abstract: Bull. Am. Phys. Soc. 54, W27.00014 (2009).
- *Magnetic Properties of High-Surface-Area Carbons & their Effect on Adsorbed Hydrogen*, J. Romanos, R. Cepel, M. Beckner, M. Kraus, J. Burress, & P. Pfeifer, 2009 March Meeting of American Physical Society, Pittsburgh, PA, March 16-20, 2009. Abstract: Bull. Am. Phys. Soc. 54, W27.00009 (2009).

Materials for H_2 Storage



possible enhancement if
E_B ~ 12 kJ/mol (5-10% B:C)