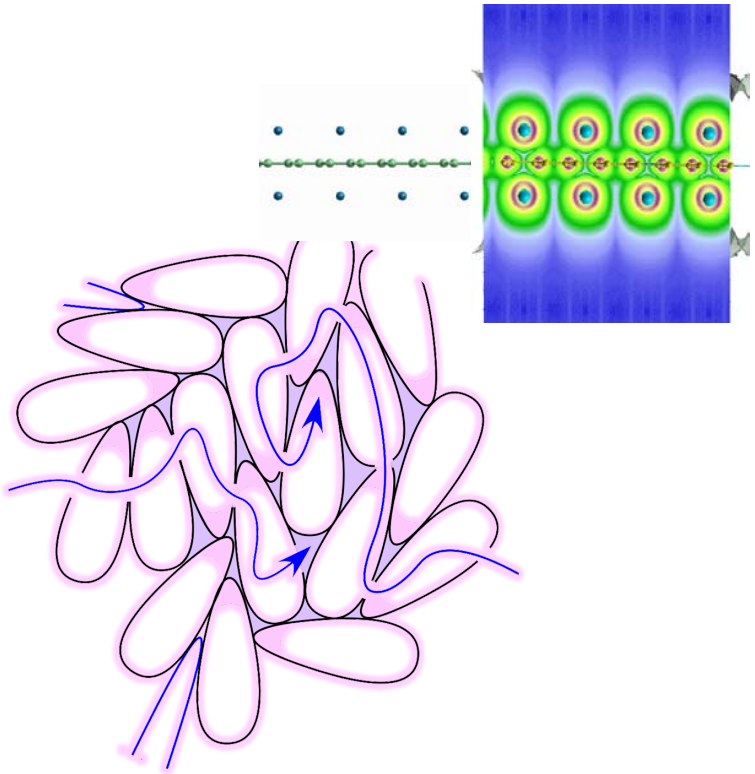
Single-Walled Carbon Nanohorns for Hydrogen Storage and Catalyst Supports

David B. Geohegan, PI
Alex Puretzky, Chris Rouleau, Mina Yoon, Norbert Thonnard, Karren More and Gerd Duscher

Materials Science and Technology Division, Center for Nanophase Materials Sciences, SHaRE User Facility, And the University of Tennessee

Oak Ridge National Laboratory, Oak Ridge, TN



Project ID ST017

DOE Hydrogen Program Annual Merit Review, June 9, 2010

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Overview

Timeline

- Project start date: FY05
- Project end date: Oct 2010
- 90 % complete

Budget

- Total project funding
  - DOE share 1.9 M$
  - Contractor share 0k
- 300k received in FY10

Barriers

- Barriers addressed
  - A. Weight and Volume
    - Reduced catalyst weight
  - B. Cost
    - Scalable production
  - C. Efficiency / Thermal Management
    - Composites
  - D. Durability / Operability
    - Catalyst stability
  - P. Lack of Understanding of Hydrogen Physisorption and Chemisorption
    - Catalyst-free production, tailorable pore sizes

Partners

- Characterization: *(Partners)*
  - Hydrogen sorption - Air Products, NREL, NIST, CalTech
  - Neutron scattering - NIST
  - NMR - UNC
  - Rice Univ. - Charged Engineered Nanospaces

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Objectives / Relevance

Overall

Utilize single-walled carbon nanohorns **(SWNHs) to understand the pore sizes and metal decoration processes needed to optimize hydrogen uptake and tune binding energy in industrially-scalable materials, such as activated carbons.**

Past accomplishments and goals

Synthesis and processing of single-wall carbon nanohorns with tunable mesopores was accomplished at high (10g/hr) rates to study effects of engineered nanospaces, and metal decoration. The material exhibits:

1) **Room temperature storage in metal-free SWNHs** - Sub-nm mesopores: 0.6 wt.% H_2 at RT (30 bar).
2) **Spillover in Pt- and Pd-decorated SWNHs** - up to 1.5 wt.% H_2 storage at RT (100 bar).

Most promising discovery and current focus – nanostructures with permanent high electric fields

A new direction for hydrogen storage resulted from theoretical predictions in this project: using metals to

1) smoothly coat carbon surfaces to take advantage of their entire surface area, and
2) create a charged surface capable of polarizing and binding hydrogen.

Alkaline earth metals (Ca, Sr, etc.) were predicted to smoothly coat nanocarbons and exhibit up to 8.4 wt.% H_2 storage at RT due to ***electric-field induced polarization***. We verified the smooth coatings of Ca.

2010 Objectives

Improve and develop Ca-coating processing techniques to uniformly coat SWNHs and other high surface-area carbons (such as MSC-30) without blocking pores. Test the theoretical predictions for increased hydrogen uptake due to electric-field induced polarization. Theoretically address the key questions for Ca decoration (e.g. effects of layer thickness, oxidation, hydride formation).

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Approach and Milestones

Task 1.Ca-decorated nanohorns and MSC-30 with high surface area

Develop activation and decoration processing approaches to Ca-decorate SWNHs and MSC-30 while preserving high surface areas. Previous approaches sacrificed surface area, but showed enhanced hydrogen adsorption relative to undecorated SWNHs of the same surface area.

Theoretically address Ca decoration processing conditions. Ab initio thermodynamic calculations of the effects of calcium layer thickness on hydrogen binding. Also oxide and hydride formation energetics for Ca bound and unbound to C.

Milestone Achieved

Increase and compare the surface areas in activated and Ca-decorated SWNHs and MSC-30 to 1000 m^2/g, and demonstrate hydrogen uptake greater than that for pure carbon material of the same surface area. *(quantitative milestone)*

Milestone Achieved / in Progress

Calculations of optimal temperature for decoration of uniform calcium coatings on carbon surfaces with and without oxygen groups, including considerations of edge states vs. surface states. Calculated effects of Ca layer thickness on optimal hydrogen binding through a comparison of the chemical potential between polarization-induced dihydrogen and chemisorbed hydrogen in calcium hydride.

Funding Decision

Go/No-Go Decision

Can MSC-30 (commercial activated carbons relevant to the Engineering Center) be coated and exhibit Increased hydrogen uptake? If so, and funded for Subtask 2 (scaleup) – downselect to MSC-30 vs. SWNHs.

Task 2.Scaled activation/decoration of Ca decorated nanohorns vs. MSC-30

Modify apparatus and approach for the scaled activation/deoxidation and Ca-decoration of downselected material. Demonstrate the scale-up approach with the production of grams quantities per run, and provide the scale-up strategy for kilogram quantities.

Theoretical calculations of pressure effects on Ca cluster dissociation.

Milestone (If funded)

Grams quantities of decorated materials demonstrated.

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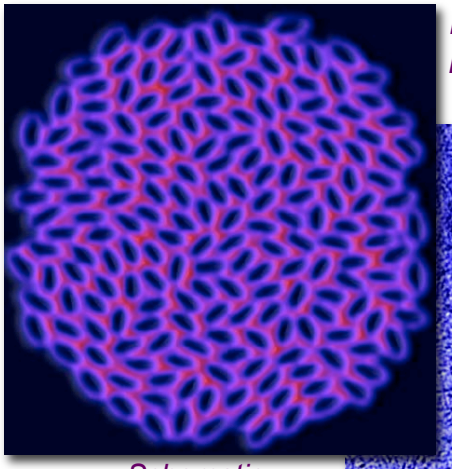
Synthesis and Processing of Ca-Decorated SWNHs and MSC-30

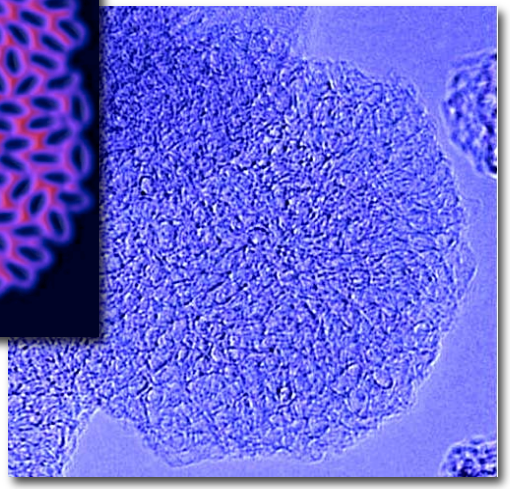
Bottom-up synthesis approach: SWNHs

- **Tune the shape of individual nanohorns during synthesis to find morphologies with adsorption sites & high binding energy (e.g. in tips of SWNHs)**
- **These nanohorns form aggregates with interstitial pores. Activate these aggregates to tune the interstitial pores and access the internal pores.**



Schematic

Packing of short SWNHs - Pore size depends on unit size and shape



TEM of short SWNH aggregate

Enhance binding through electric-field induced polarization mechanism: Post processing by metal decoration:

- **Focus on our theoretical prediction (also substantiated theoretically by others) that Ca-decorated carbon nanostructures (including graphene, fullerenes, nanotubes, etc. should exhibit strong binding and hydrogen storage at room temperature from 6 - 8.4%)**
  Focus on experimental demonstration.
- **Expand materials to include high-surface-area activated carbons such as MSC-30.**
  Can commercial activated carbons be post-processed to improve their room temperature hydrogen adsorption simply by Ca-decoration?

H_2

Ca

C

$5H_2$ per site:
$\Delta E \sim 0.4$eV per H_2

Each Ca atom is bonded to a surface carbon site and can bind up to 5 dihydrogen.

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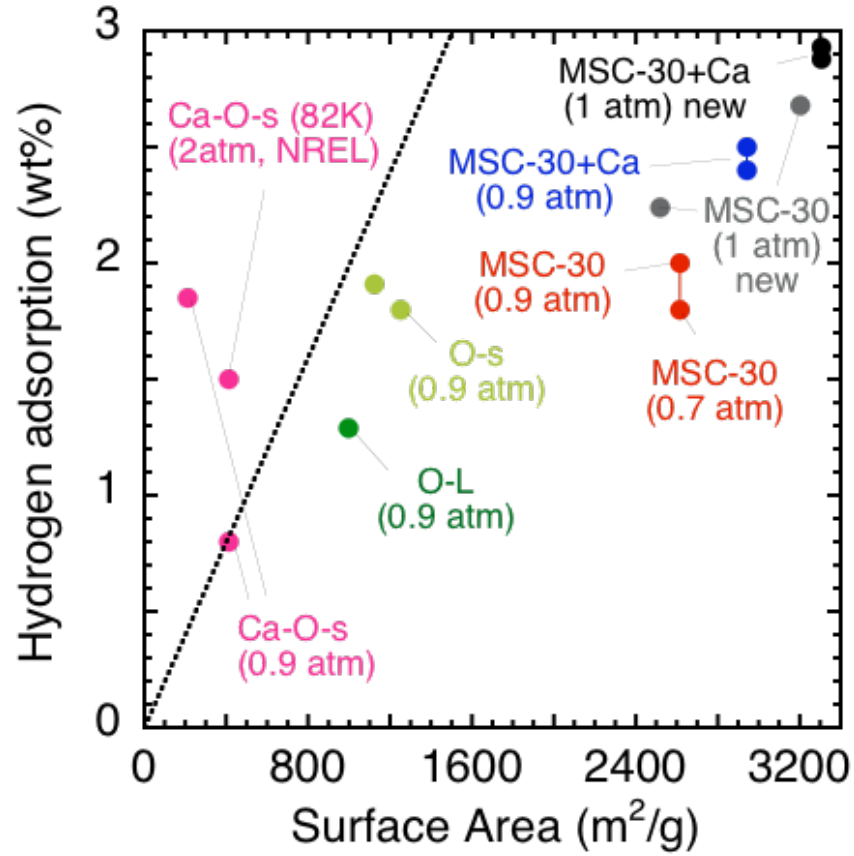
Technical Accomplishment

Low pressure excess hydrogen adsorption in Ca-Decorated carbon nanostructures materials at 77K: SWNHs and MSC-30

Material	H_2 wt%	@ P (atm) H_2	N_2 BET surface area (m^2/g)	FOM (H_2 wt% per 500 m^2/g per atm H_2
S-O-SWNHs +Ca (1)	1.85	0.9	212	4.8
S-O-SWNHs +Ca (2)	0.8	0.9	413	1.1
S-O-SWNHs (1)	1.9	0.9	1123	0.94
S-O-SWNHs +Ca (2)	1.5	2	413	0.91
S-O-SWNHs (2)	1.8	0.9	1251	0.80
L-O-SWNHs	1.3	0.9	997	0.72
AX21	1.8	0.7	2615	0.49
AX21+Ca	2.5	0.9	2942	0.47
AX21+Ca	2.4	0.9	2942	0.45
AX21	2	0.9	2615	0.42

- Ca-decoration of oxidized short SWNHs and MSC-30 activated carbon were performed by high-temperature vapor infiltration in vacuum, and compared to undecorated samples.
- Although pore-blocking was observed by nitrogen BET, the hydrogen storage capacities at ~ 1 atm. in Ca-decorated samples already exceed those expected by Chahine's rule (see graph at right, and Figure of Merit (FOM) above).
- Interesting, reversible hydrogen isotherms at 77K indicate possible capillary filling

Summary of low-pressure (~ 1 atm.) 77K excess H_2 adsorption results



Ca decoration results in clear enhancement of hydrogen adsorption even at highly reduced surface areas. The decoration process should be improved to preserve the surface area of nanostructured carbon.

AX-21 Courtesy of CalTech (actual description MSC-30)

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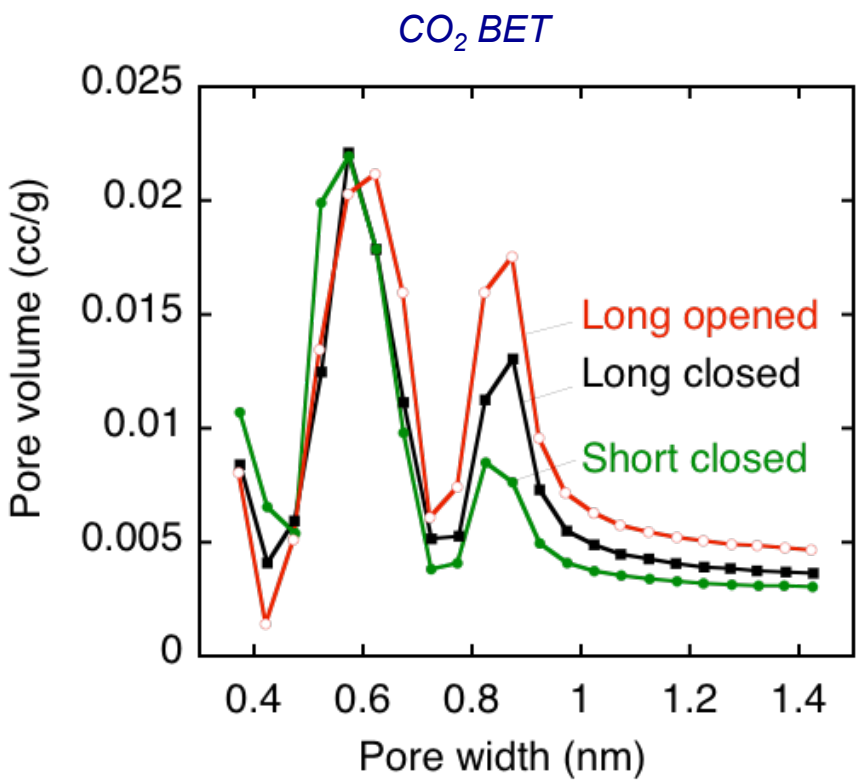
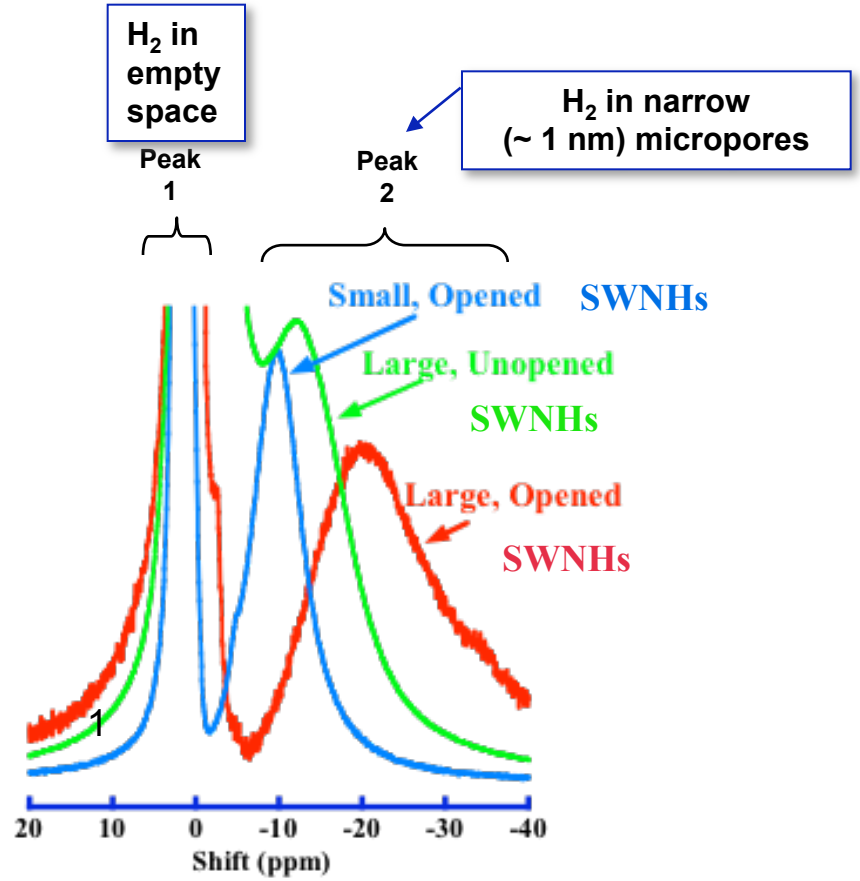
Sub-nanometer pores in activated SWNHs





Peak shift for smaller pore size

CO_2 pore size distributions were measured and correlated with NMR shifts measured at UNC which reveal which pores store hydrogen in large and small SWNHs, before and after oxidation. The results indicate that the smallest pores (0.5 – 0.7 nm) are not as active as the pores in the 0.8-1.0 nm range in storing hydrogen.

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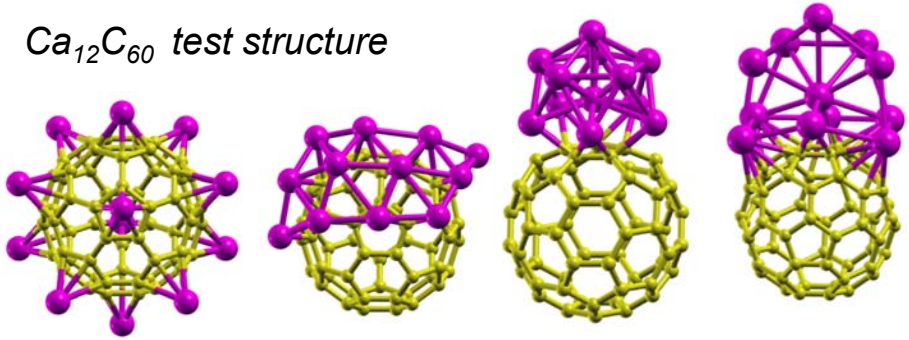
Calculations of Ca-Coating – Implications for Ca Processing and H_2 Storage

Energies of different 2D and 3D systems were calculated and compared.

Will Ca form a single layer or form a cluster?

The smooth atomic layer is the most energetically preferred configuration. 2D layers are more favorable than 3D.

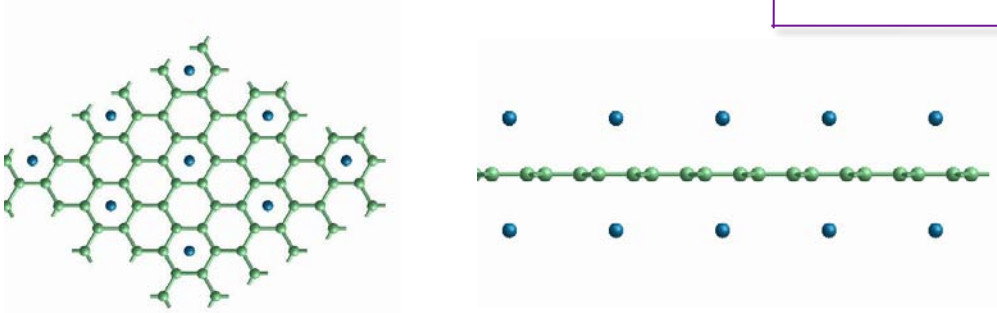
$Ca_{12}C_{60}$ test structure



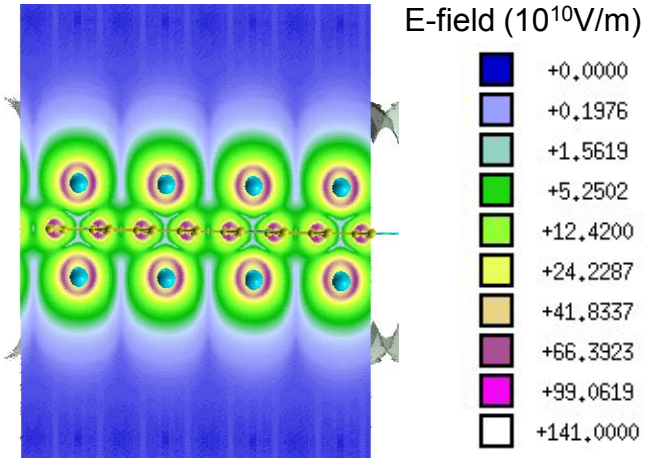
Homogeneous	2D layer	3D cluster 1	3D cluster 2
+4.81 eV	**-0.67 eV**	**0.0 eV**	**+0.70 eV**

(Total E with respect to the 3D cluster1 structure)

Can both sides of a graphene surface (or activated nanohorn) be Ca-coated and used for hydrogen storage?



Ca atoms on both sides of graphene polarize and bind hydrogen molecules by electric field-induced polarization just as effectively as Ca atoms on just one side.



Ca atoms should form atomically smooth 2D layers, and both sides of graphene can be used to polarize and bind hydrogen by simple Ca decoration

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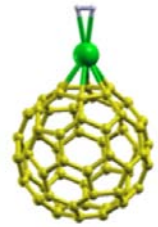
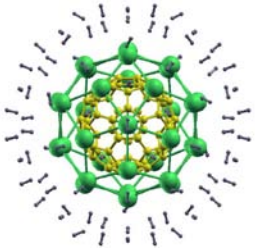
Calculations of Hydrogenation on Ca-Coating

Our study indicates that H_2 dissociation cannot occur on Ca-decorated graphene or Ca-decorated fullerene surfaces without any thermal effects

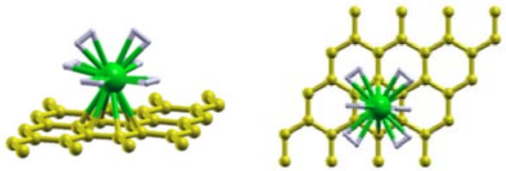
[Phys. Rev. Lett. 100, 206806 (2008), M. Yoon et al.]



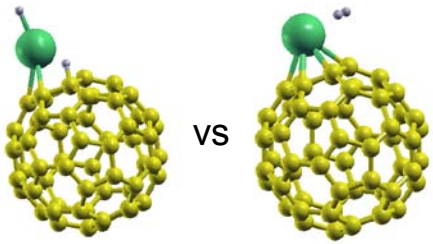
H_2 on CaC_{60}



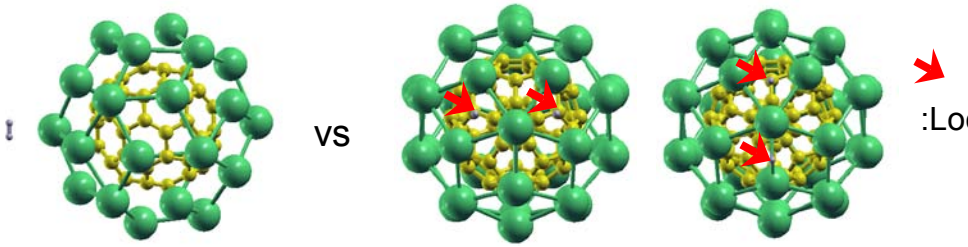
H_2 on $Ca_{32}C_{60}$



H_2 on Ca decorated graphene



vs



vs

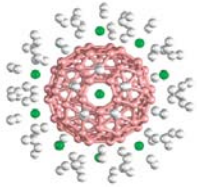
:Location of H

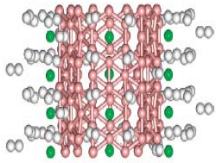
Dihydrogen state is more favorable by 0.47eV/H

Hydrogenated state is more favorable by 0.66eV/H

We will further study thermodynamics and kinetics of H_2 dissociation processes at a finite T

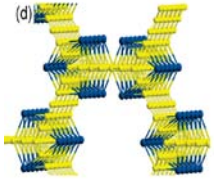
Studies on other systems also support our finding: No H_2 dissociation on Ca surfaces at T=0

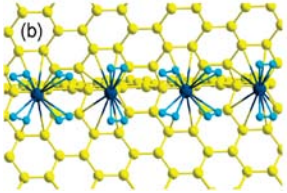




H_2 on $Ca_{12}B_{80}$ H_2 on Ca-B(9,0) tube

[Nano Lett. 9, 1944 (2009), M. Li et al.]





H_2 on Ca-decorated graphene-based 3D

[J. Phys. Chem. C 113, 20499 (2009), G. Kim and S.Jhi]

Many studies have shown that hydrogen molecules are adsorbed on Ca-decorated carbon surfaces without dissociation at T=0

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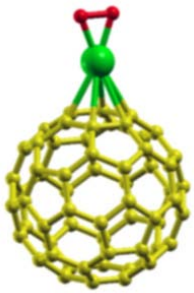
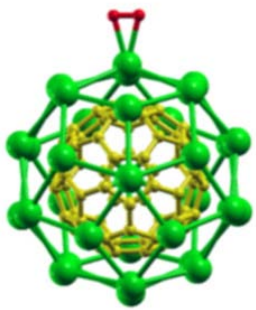
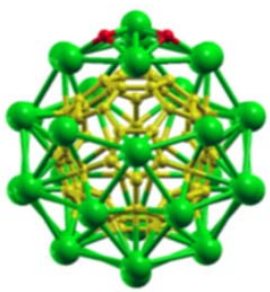
Calculations of Oxidation on Ca-Coating



No immediate dissociation of O_2 on CaC_{60}

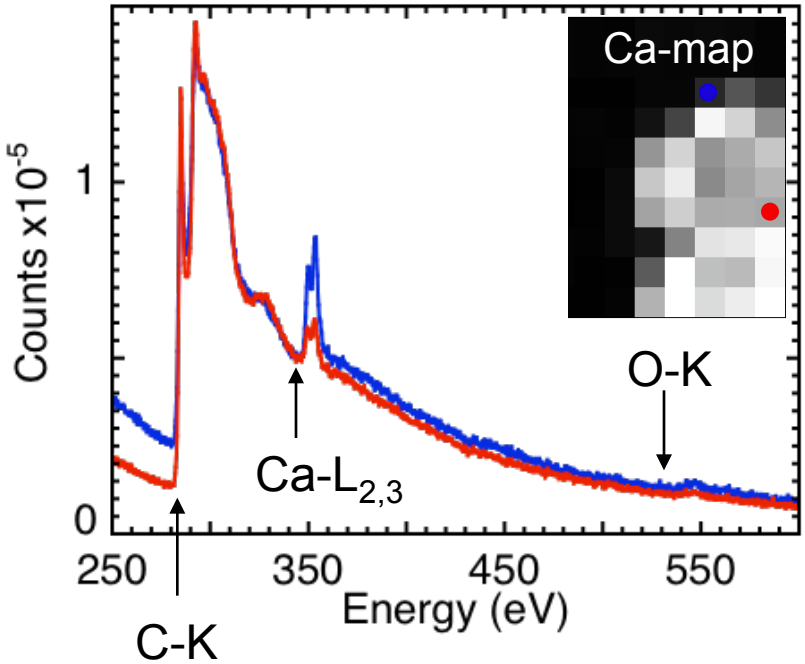


initial configuration



final configuration after full structure relaxation

EELS spectra of Ca-decorated nanohorns



Some oxygen observed in Ca-decorated SWNHs (which were transferred quickly through air to the TEM)

O_2 can oxidize on Ca monolayer surface even at T=0.
There is no barrier for O_2 dissociation. So must avoid oxidation of decorated material.

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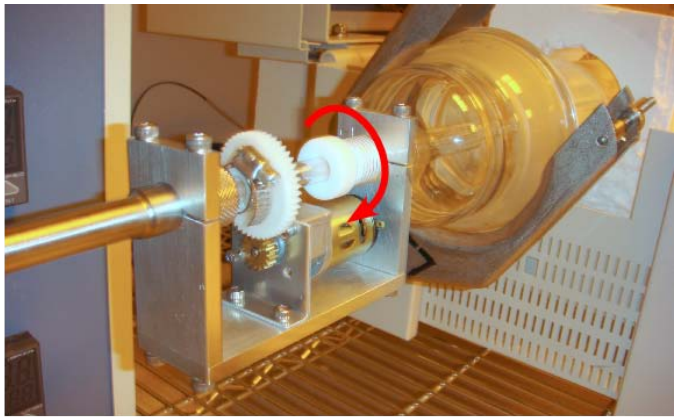
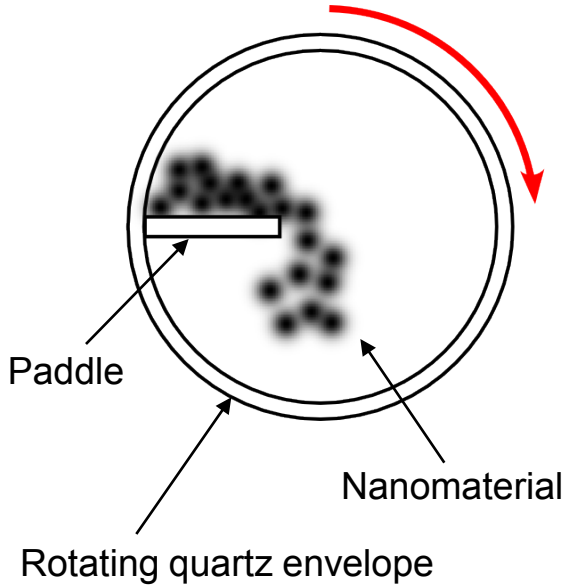
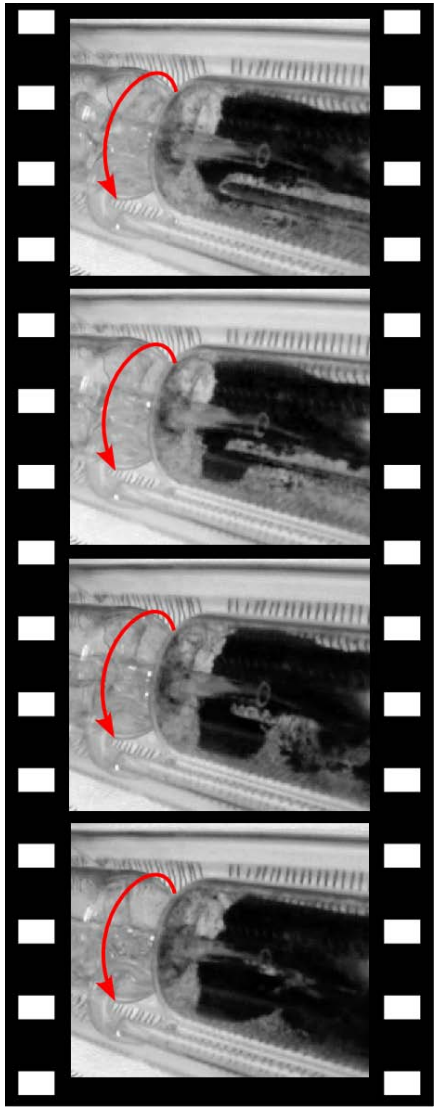
Developing more uniform activation strategies for higher surface areas







- **Simple, scalable gas phase process**
- **Direct injection of flow gas for more uniform flow currents**
- **Continuous agitation for uniform exposure to oxidant gas**

New activation approach was developed to activate carbon nanomaterials and increase their surface areas

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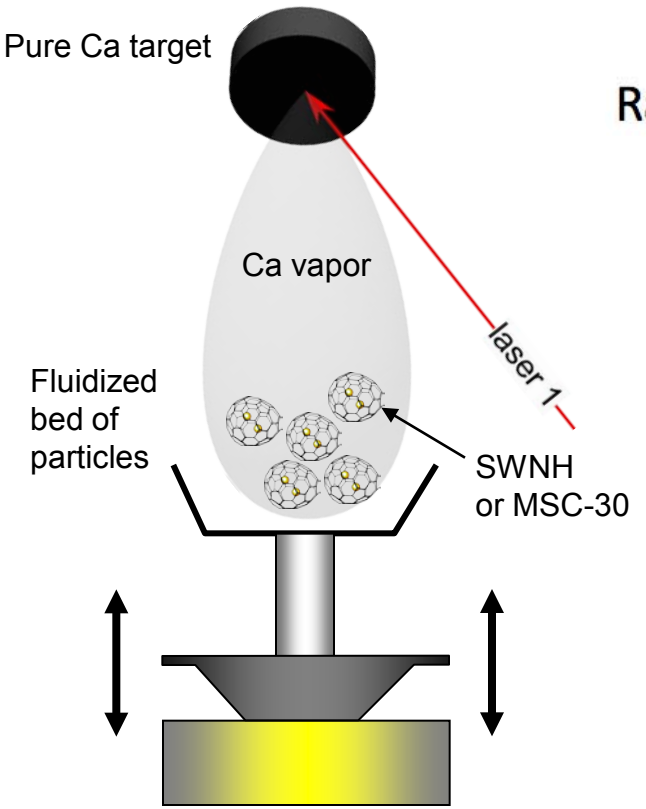
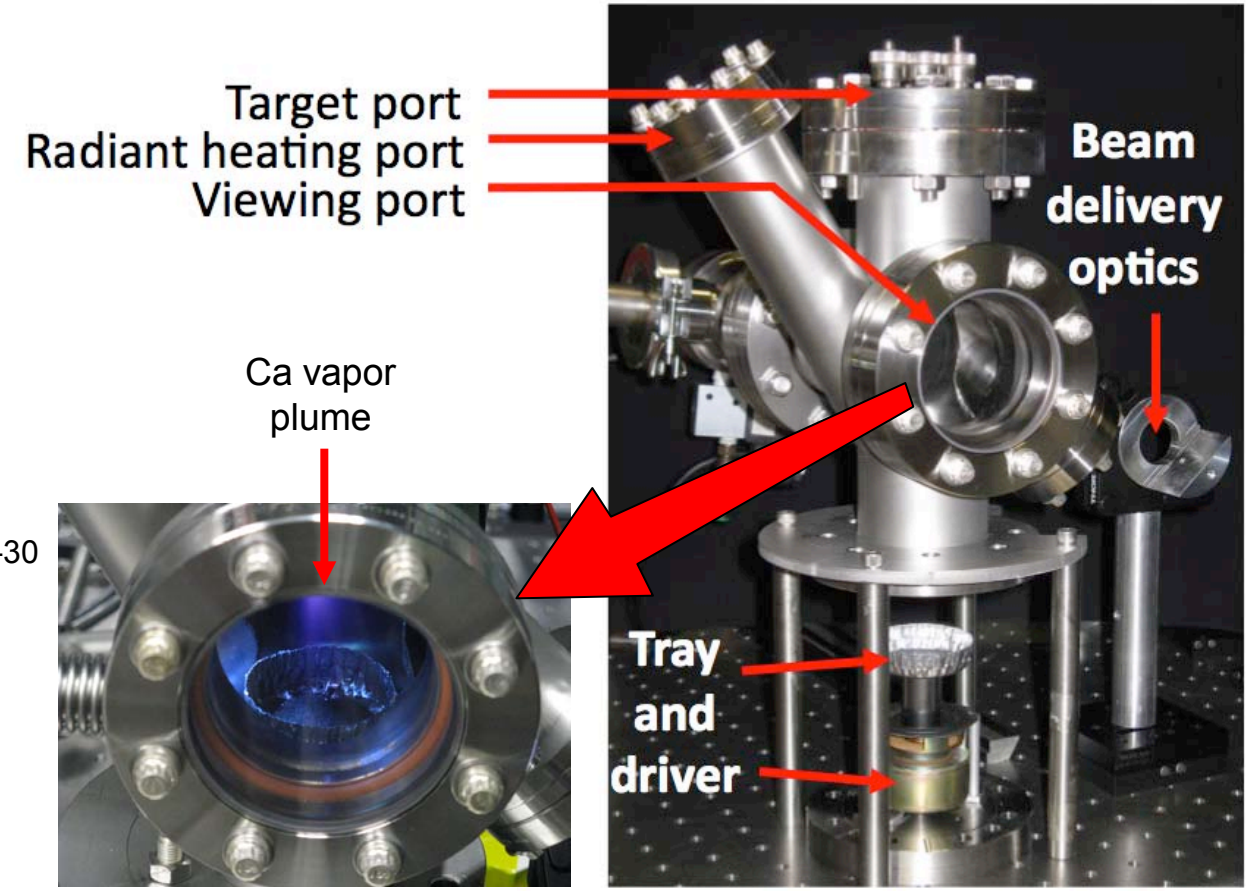
Developing scalable strategies for Ca decoration of nanocarbons





Large quantity powder coating chamber with processing station removed for clarity

A vacuum pulsed laser deposition method to coat and preserve against oxygen exposure ~ 200 mg quantities of fluidized MSC-30 or nanohorns with high-kinetic energy calcium vapor was developed and demonstrated

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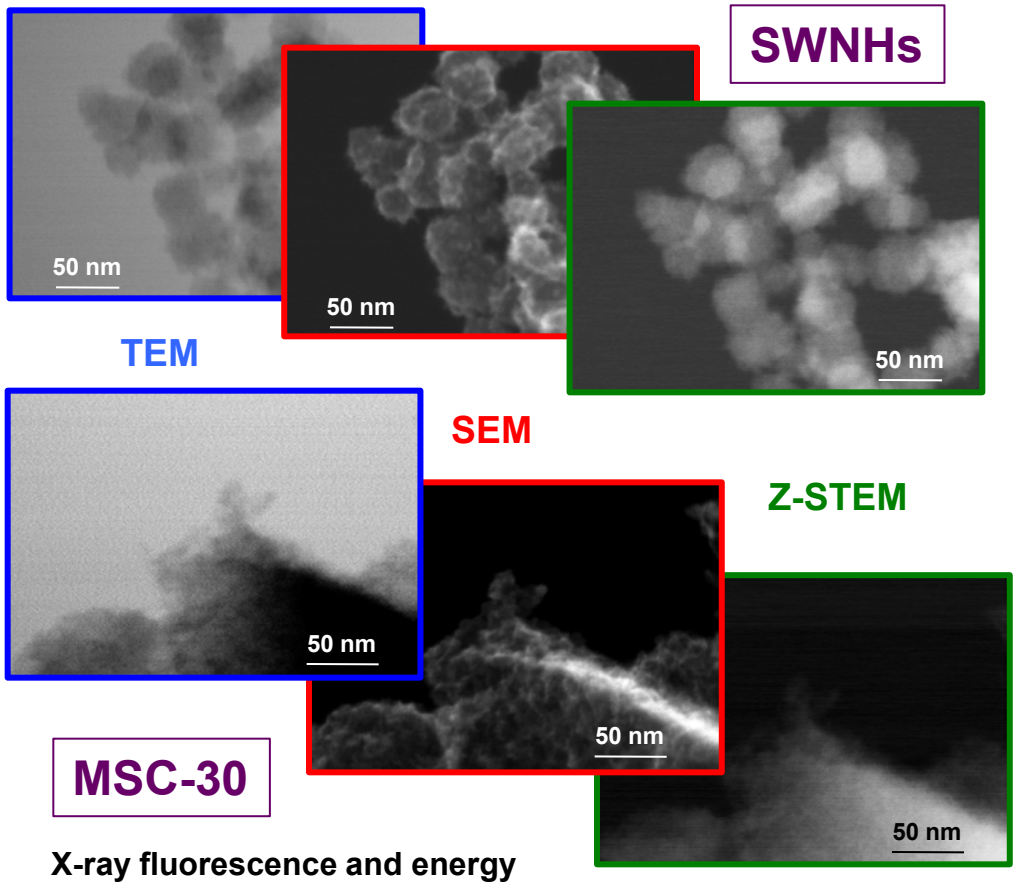
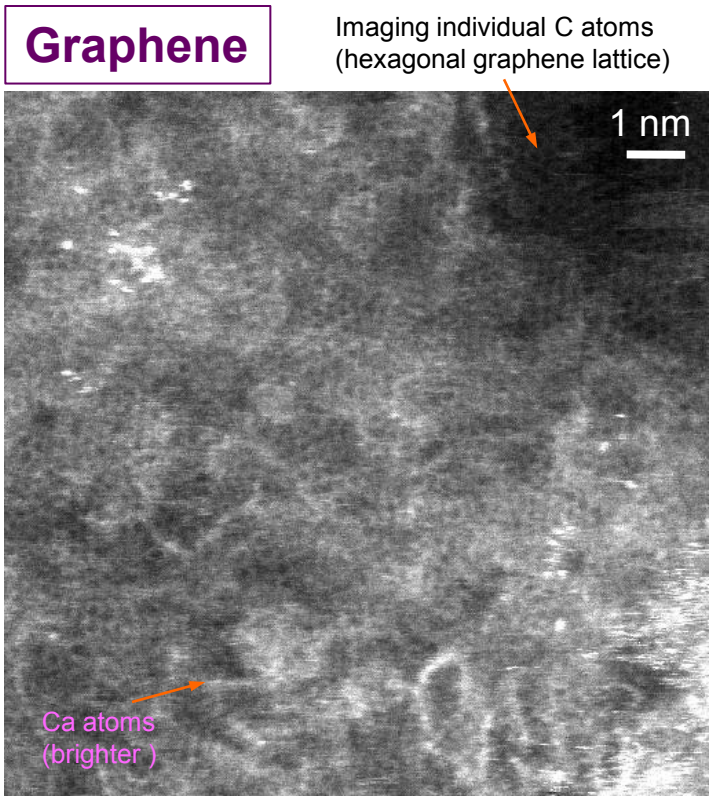
Testing Predictions of Atomically Thick Coatings by Ca-decoration



X-ray fluorescence and energy dispersive x-ray analysis indicate deposited Ca which scales linearly with deposition time



Preliminary ultra-Z-STEM images (courtesy Matt Chisholm, ORNL) of Ca-decorated graphene flakes (showing atomic layer Ca thicknesses and edge decoration morphology) but no nanoparticles of Ca. Graphene was synthesized by Murari Regmi and Gyula Eres at ORNL.

The morphology of Ca-decorated SWNHs (upper), Ca-decorated MSC-30 activated carbon (lower), and Ca-decorated graphene (right) indicate smooth, nanoparticulate free coatings in agreement with theoretical predictions. Ca appears to decorate edges of graphene flakes.

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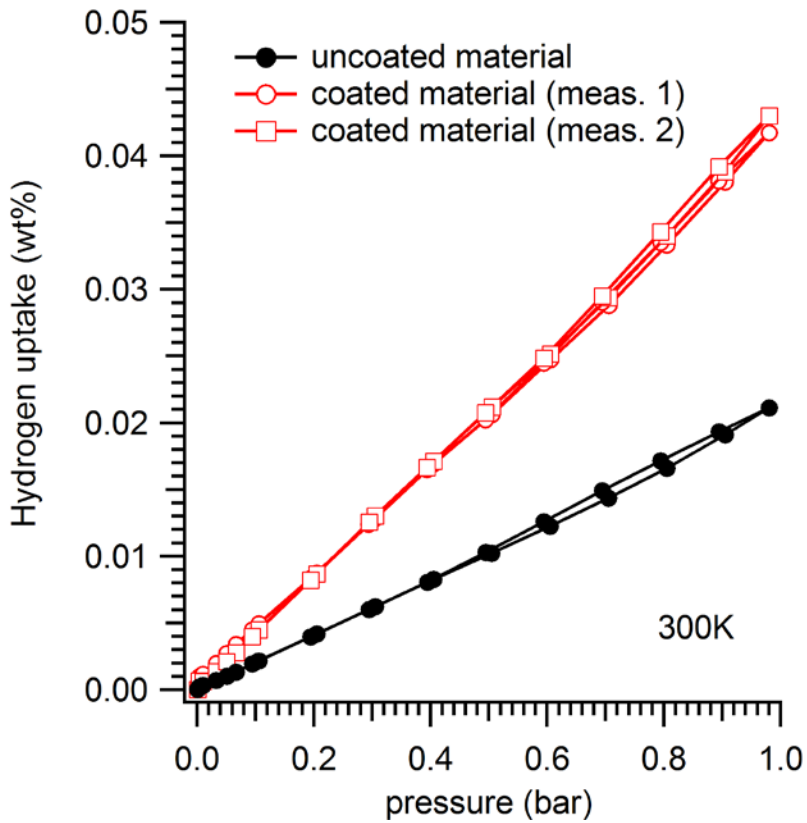
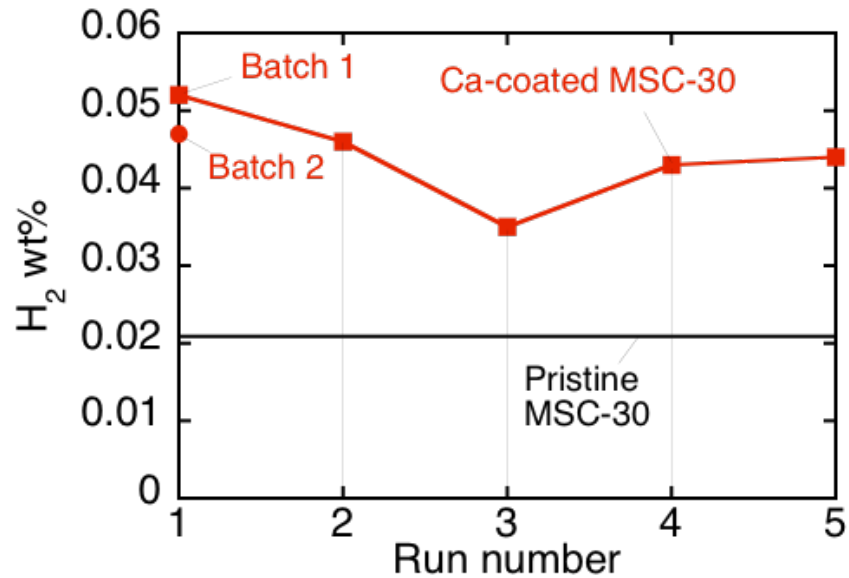
Improved room-temperature uptake in Ca:MSC-30 vs. MSC-30



Consecutive cycles of same batch



Hydrogen uptake at room temperature in Ca-coated (red curve) and uncoated MSC-30 activated carbon. The Ca coated material shows a factor of 2 improvement. Both materials had ~ 3300 m^2/g N_2 BET surface areas, which is the consensus value for this material, indicating that coating did not block the pores in the virgin MSC-30.

Significant enhancements in the reversible, room temperature adsorption of MSC-30 were measured at room temperature at 0-1 bar in Ca-coated MSC-30 yet reproducible batch to batch. Atomic resolution imaging of the materials is ongoing to determine the optimal coating morphology and chemistry.

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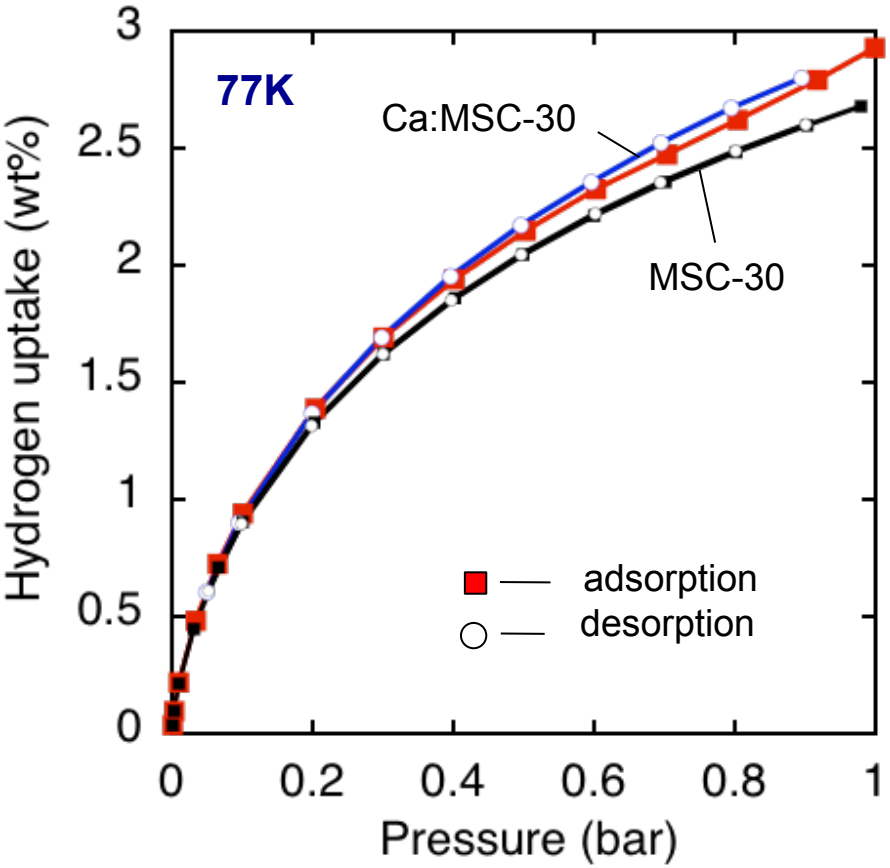
Low temperature hydrogen adsorption in Ca:MSC-30 vs. MSC-30



Material	H_2 uptake, wt%, at 1bar, 77K	N_2 BET, m^2/g
Ca-coated MSC-30	2.93 2.88	3306 3306
Pristine MSC-30	2.68 2.24	3204 2519

At 77K Ca-coated MSC-30 shows only modest ~10% improvements in hydrogen uptake at 1 bar compared with pristine MSC-30 of the same surface area. Ca coating appears to *increase* surface area slightly, possibly acting as a getter.

The lack of enhancement at 77K and the > 200% enhancement at room temperature implies an activation energy barrier for attachment of hydrogen to Ca coated MSC-30.

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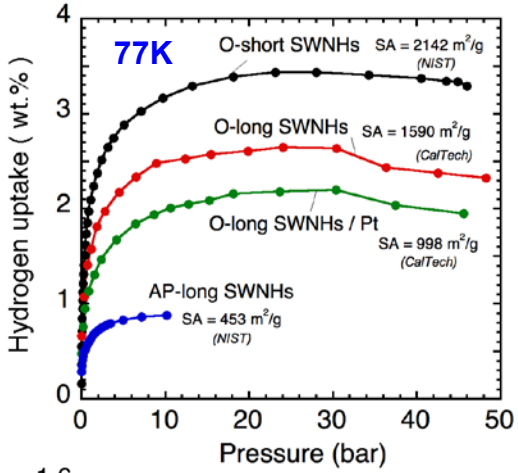
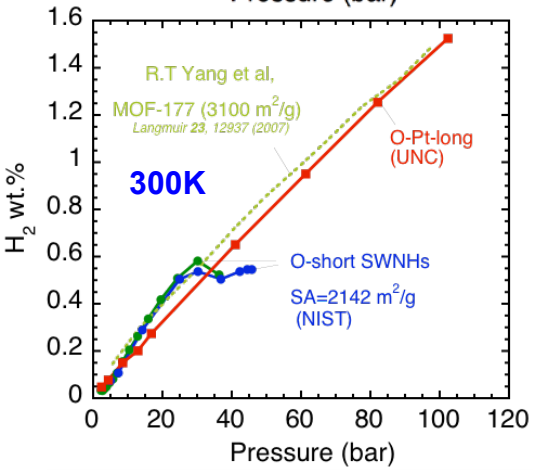
Collaborations

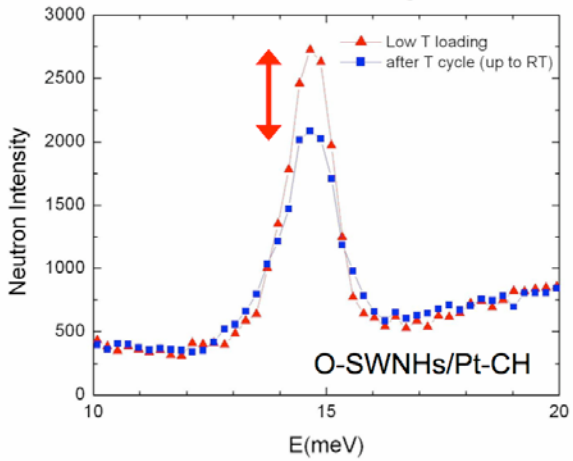
Hydrogen uptake measurements by Air Products (API), NREL, NIST, CalTech, and UNC

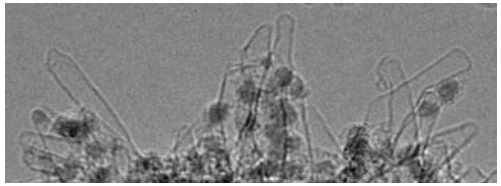




Short O-SWNHs adsorb 0.6 wt.% at RT and 30 bar, comparable to bridged MOFs

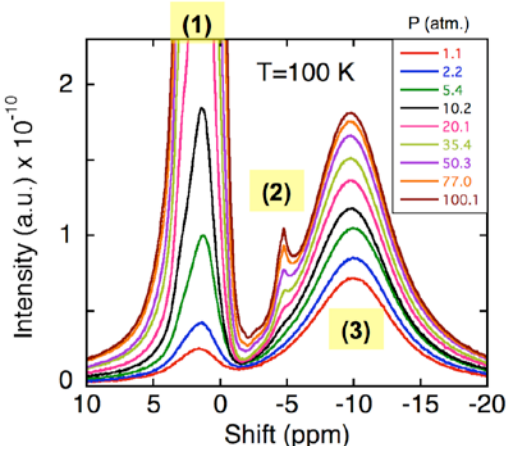
Neutron scattering measurements by NIST

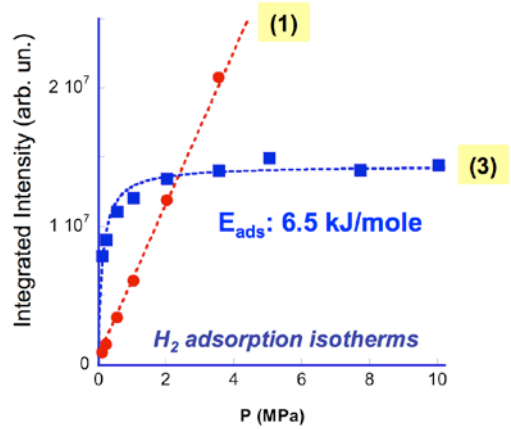




"Spillover" measurements confirm that Pt-decorated SWNHs dissociate H_2 with an onset temperature between 150K < T < 298K.

NMR measurements by UNC





Short opened SWNHs store hydrogen nearly entirely within pores which are optimally sized (< 1 nm).

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Proposed Future Work

This project has developed a new concept of nanoscale architectures which maintain electric fields sufficient to polarize and bind hydrogen. One architecture is Ca-decorated carbon, which forms an electric field around the entire surface of the decorated C, and appears to be very promising since the demonstrated effect extends to commercial carbons. Clearly, pursuing the design and synthesis of other inexpensive materials, such as ionic organic crystals or thin films, with high, built-in electric fields is a future direction of research.

This year FY2010

Continue to focus on Ca-decorating activated carbons and nanohorns because some low-pressure isotherms indicate a large **(>2X)** enhancement in the reversible hydrogen storage ***at room temperature*** (but not 77K) due to Ca-decoration of MSC-30 activated carbon. The limits of this effect have not been quantified. Understand the origin of the effect through atomic-resolution microscopy and modeling. Produce more material and obtain high-pressure isotherms and binding energies. Implement online process diagnostics to quantify Ca deposition process.

Milestone – Go / No-Go – Scaleup – FY2010-FY2011

A milestone decision on whether to proceed with an additional task (and additional funding) in this project occurs now. A Go / No-Go decision whether to scale-up the production of Ca-decorated (a) SWNHs or (b) activated carbon decoration is required. If the factors of two in hydrogen uptake through Ca-decoration and processing can be extended to high tank pressures, then scale-up to larger quantities is obviously warranted.

Future

This project has shown a path forward through the *atomistic design and screening* of nanoscale materials with high, built-in electric fields, capable of polarizing and binding hydrogen. Based upon the work herein, the Ca-decorated nanocarbon system looks extremely promising, is the focus of ongoing worldwide research, and processing / testing of this material in scaled volumes should continue to be pursued in this project. Other systems, such as organic crystals, should also be pursued.

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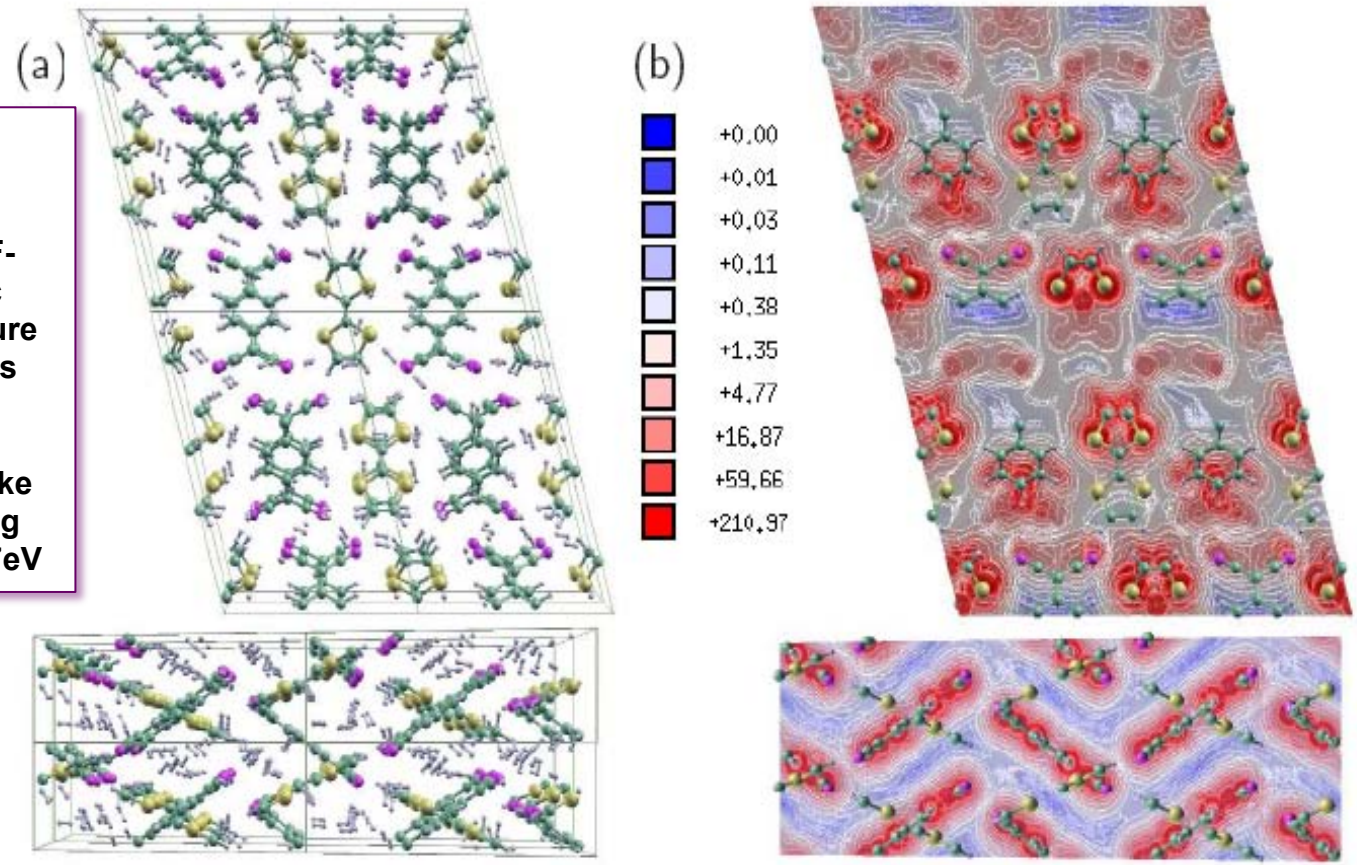
Proposed Future Work: Charge Transfer Organic Crystals

Results of calculations showing fully optimized TTF-TCNQ organic crystal structure which includes the predicted 7.7wt% and 8.2g/L H_2 uptake with H_2 binding energy of 0.17eV



Electric fields within the crystal are in units of 10^{10} V/m (see scale at left) and illustrate the areas where H_2 molecules are strongly bound.

In charge-transfer organic crystals, high electric fields exist naturally which provide the mechanism for binding H_2 without introducing any additional metal atoms. These materials should be explored for systems which are inexpensive, self-assembling, and of the right lattice parameters for storing large quantities of H_2.

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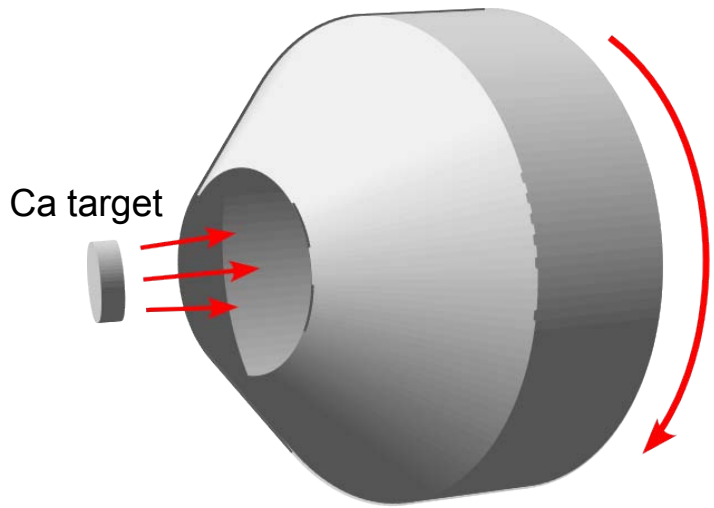
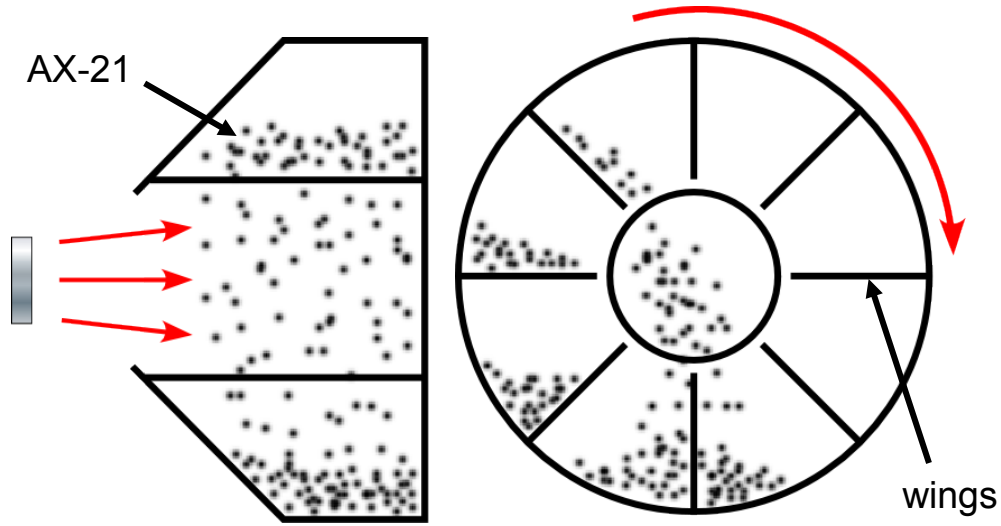
Proposed Future Work: Scaling Ca Decoration of AX-21





A rotating wing drum has been shown to provide an effective means of increasing homogeneity during surface modification[1] and coating of powders,[2] and is amenable to a variety of physical vapor sources, including pulsed laser ablation and sputtering.

Powder grains are lifted by the wings of the rotating drum, and dropped through the deposition beam on a continuous basis, thereby providing a great deal of statistical uniformity.

[1] *Rev. Sci. Instrum.* **65**, 2963 (1994).

[2] *Surface and Coating Technology* **163-164**, 281 (2003)

Ca decoration can be scaled-up using existing approaches and their modifications

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FY10 Summary

Focus: Testing our theoretical predictions that Ca-decorated carbon should bind dihydrogen due to a high surface electric field. Last year, we observed anomalous storage in Ca-decorated SWNHs and MSC-30, but pore blocking was a problem, reducing surface area. New efforts to activate and decorate materials needed to be developed, and confirmation of the theoretically-predicted smooth coating needed to be made. If the theoretical predictions were true, this points toward a new direction in hydrogen storage, nanostructure architectures with high permanent electric fields.

- **Achievements**
  - ***Processing***: New methods for activation by gas-phase oxidation, and uniform coating of nanomaterials were developed.
    - ***Activation***: A rotating, tumbling reactor was developed and tested to more uniformly activate nanohorns.
    - ***Ca-Coating***: Several methods were explored to uniformly coat nanohorns and commercial activated carbons such as MSC-30 with calcium vapor. A mechanically-agitated fluidized bed, coupled with pulsed laser deposition of calcium vapor in vacuum was shown to produce highly uniform calcium coatings on SWNHs, MSC-30 and graphene films. Calcium appeared highly uniform and well distributed in SEM, TEM, and Z-STEM images, however ultra-Z-STEM imaging of individual atoms indicates Ca may move to edges of graphene flakes.
  - ***Room temperature storage***: Room temperature excess storage in 3300 m^2/g MSC-30 activated carbon was enhanced more than 200 % to 0.05 wt.% at 1 bar. The effect was highly reversible, and highly reproducible within a batch. Run to run variations between coating runs were observed and have not been explained yet. The enhancements did not occur at 77K, indicating a thermally-activated process (similar to that observed in Pd- and Pt-decorated SWNHs).
  - ***Pore sizes responsible for room temperature storage in short-SWNHs:*** We measured the sub-nm pore size distributions in short and long nanohorns, and in work with the University of North Carolina which reveal which pores are storing hydrogen using NMR, concluded that the smallest pores (5-7 Å) are likely not participating, and that the 8-10 Å pores are largely responsible.
- **Future Work and Go/No-Go recommendation:** Encouraging room-temperature storage enhancement in Ca-decorated MSC-30 activated carbon warrants further investigation. If enhancements are reproduced at high pressures in test samples, other materials such as PEEK and SWNHs should also be investigated. Scaled coating technology should then be pursued, along with ultra-microscopic investigations of the mechanism in concert with theory.

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Supplemental Slides

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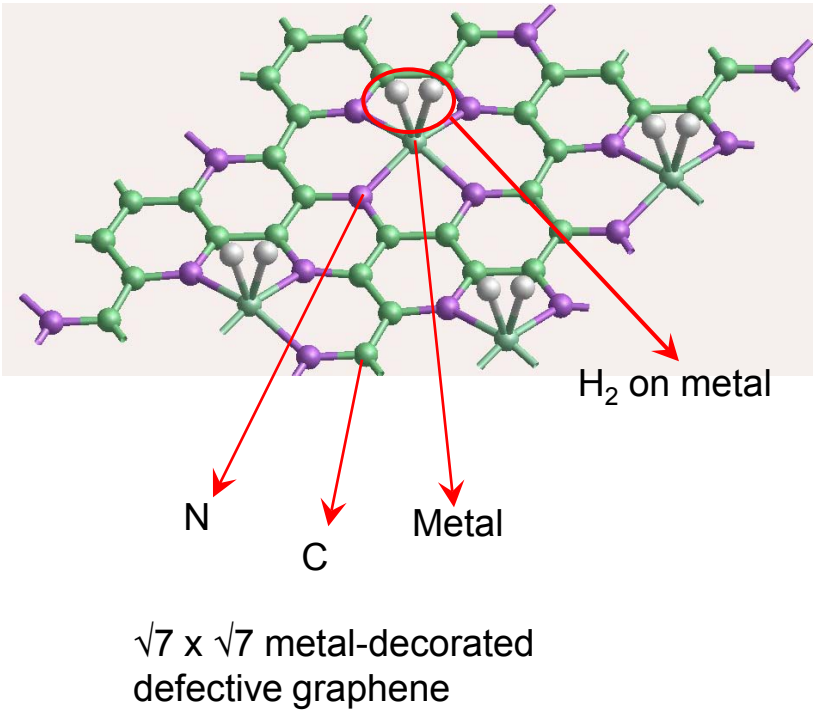
Calculation Method: Dihydrogen Binding Strength to Metals

H_2 binding energy values from ab initio density functional calculations:
exchange-correlation energy dependence – LDA vs GGA?
Importance of zero-point energy contribution?

	H_2 binding energy on √7 x √7 porphyrin-incorporated graphene **Values in parentheses: including zero-point energy contribution**	
	GGA (PBE) (eV)	LDA (eV)
Ti	0.26	0.70
V	0.140 (**0.042**)	0.585 (**0.460**)
Ca	0.059 (**-0.019**)	0.173 (**0.095**)
Mg	0.035 (**-0.041**)	0.163 (**0.086**)
Zn	0.013 (**-0.058**)	0.105 (**0.030**)

Example: Porphyrin-incorporated graphene



- **Difference in H_2 binding energies from LDA and GGA calculations can be as large as ~0.4eV**
  → The "true" binding energy lies in between LDA and GGA values
  (High level calculations are necessary for comparison)
- **It is very important to include zero-point energy contribution, in particular for physisorption case**
  → zero-point energy contribution is as large as 100% of H_2 binding energy

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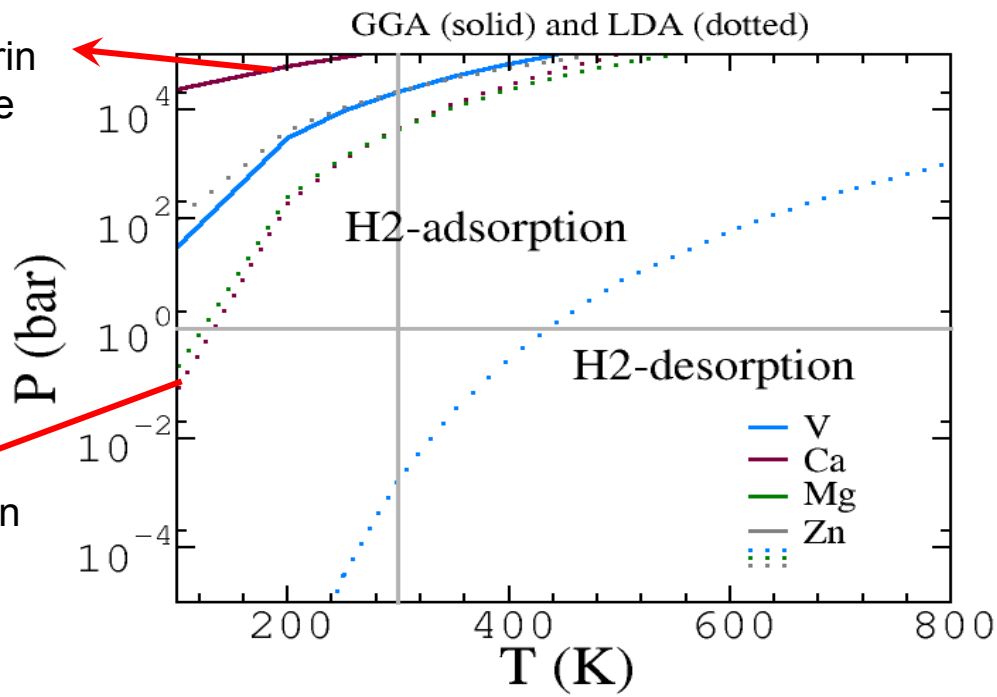
Calculation Method: Construction of H_2-adsorption/desorption phase diagram

Example: Porphyrin-incorporated graphene

Ca-containing porphyrin incorporated graphene (GGA)

Ca-containing porphyrin Incorporated graphene (LDA)



Each line identifies the thermodynamic phase boundaries for H_2 adsorbed/desorbed regimes

Regions above Lines: H_2 adsorption condition
Regions below Lines: H_2 desorption condition

Low H_2 binding energy: High P is required to adsorb H_2
High H_2 binding energy: Low P is required to desorb H_2

- **Ab initio thermodynamics approach is performed to construct the phase diagram**
- **Among the considered metals V is most promising, where H_2 operation is possible at the experimentally accessible P & T conditions**
- **We expect that Ca-decorated graphene (which has close binding energy to that of V-incorporated structure) has promising T & P condition for H_2 operation**

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Overall Program Summary

- **Overall:** This program has demonstrated that pore sizes in carbon nanohorn aggregates can be tuned 1) during synthesis, and 2) during activation , and that this sometimes results in room-temperature binding of up to 1.5 wt.% hydrogen. The effects of metal decoration have been demonstrated. Clear spillover and enhanced binding energy were observed. Decoration with Ca has been shown to result in smooth nanoparticle-free coatings and anomalously high storage, in agreement with our proposed mechanism of *polarization induced by high local electric fields* resulting from the alkaline-earth metal "doping" of C by decoration. Significant enhancements in room-temperature storage at 1 bar have been demonstrated for MSC-30 activated carbons by coating with Ca.

- **Nanohorns: Summary of results**
  - *High surface areas*: SWNHs were synthesized in gram quantities with pore sizes adjusted to maximize surface area (2142 m^2/g) and increase excess storage (3.5 wt. % at 77K).

  - *Tunable, small pores*: NMR confirmed the majority of storage in the interstitial (~ 0.5 nm) pores on large SWNHs, and in activated pores (< 1 nm) in short-SWNHs. These NMR shifts are the highest among all materials studied, indicating storage in very small pores. Work continues to understand the activation process, but is aided by the stability of the nanohorn aggregate structure which is defined at very high temperatures during synthesis.

  - *Room temperature storage*: Undecorated, short O-SWNHs reversibly store significant hydrogen (0.6 wt.% at 30 bar) at room temperature, comparable to bridged MOFs and Pt-decorated O-SWNHs (1.5 wt.% at 100 bar). These "nanoengineered pores" are defined both by the unique nanostructure self-assembled during synthesis, and by the activated pores during oxidation. Decoration with

  - *Enhanced Binding Due to Metal Decoration - Doping-Induced Charge Separation -* Methods of vapor phase Ca-decoration were developed and found to result in smooth decoration (unlike decoration by transition metals which results in small nanoparticles). These results confirm our theoretical predictions, which predict that of all the elements, alkaline earth metals **Ca and Sr** should have a special ability to coat C nanostructures without clustering while providing sufficient electric field strength to polarize and bind H_2 with 8.4 wt. % and 0.4 eV for Ca.

- **Program Focus: Charged nanostructures for hydrogen storage**
  - Activate and Ca-decorate O-SWNHs and commercial carbons such as MSC-30 for maximal H_2 uptake.
  - Theoretically search for new nanostructures with stable, dipole fields, such as organic molecule-based "ionic crystals"with sufficient internal spacing to store hydrogen.

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Summary Table

Different types of carbon materials		Surface area, BET (m^2/g)	Pore size (nm)	H_2 uptake at 300K (wt.%)	H_2 uptake at 100K (wt.%)	H_2 uptake at 77K (wt.%)	H_2 uptake at 30K (wt.%)
As prepared "long"	AP-SWNHs	453		0.18 (AirProd.) 0.2 (NIST)	0.6 (NIST)	1.0 (NREL) 0.8 (NIST)	1.7 (NIST)
Opened by oxidation "long"	O-SWNHs-4	1191	1.5(BET)				
	O-SWNHs-3	1590	1.7(BET)			2.5(30bar) (CalTech)	
	O-SWNHs-5	1892	1.7(BET)				
As prepared, Pt dec.,"long"	SWNH/Pt-LA			0.22 (AirProd.) 0.2 (NIST)	0.6 (NIST)	1.0 (NREL) 0.8 (NIST)	1.7 (NIST)
	SWNH/Pt-CH			0.28 (110bar) (AirProducts)			
Opened and Pt dec.,"long"	O-SWNH-3/Pt-CH					2.2(30bar) (CalTech)	
				1.5 (100bar) (UNC)			
Opened, "short"	O-SWNHs_1	2142		0.6 (30bar) NIST	2.7 (30bar) NIST	3.5 (25bar) NIST	6.3 (4bar) NIST
Opened and Ca dec. "short"	O-SWNHs+Ca	212				1.9 (0.9bar)	
	O-SWNHs	1123				1.9 (0.9bar)	
MSC-30		3204 2519		0.02 (1 bar)		2.7 (1bar) 2.2 (1bar)	
Ca:MSC-30		3306		0.05 (1bar)		2.93 (1bar) 2.88 (1bar)	

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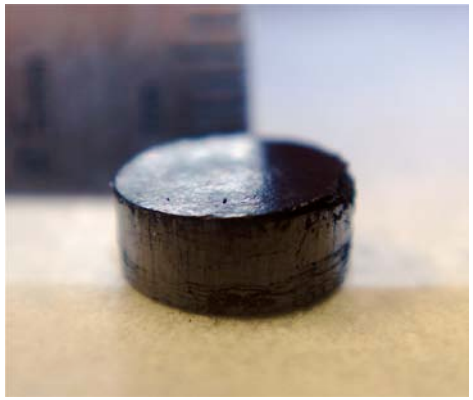
SWNHs: net gravimetric and volumetric capacities

Volumetric capacity

Volumetric capacities of 36 g/L (assuming 3.5 wt.% H_2 stored) were achieved in pure SWNHs which have been compressed to form dense pellets (1.03 g/cm^3).

Ca-decorated SWNHs with 8.4 wt.% H_2 stored should enable 86.4 g/L volumetric capacities to address 2010 (45 g/L) and 2015 (81 g/L) system targets.



SWNHs pressed pellet

Net gravimetric capacity

Experimentally, 97% of hydrogen stored in engineered nanospaces within activated SWNHs at room temperature (up to 1.5 wt.%) is released at 3 bar pressure.

The enhanced storage capacities due to Ca decoration of SWNHs (up to 8.4 wt.%) will be utilized to address 2010 (6 wt.%) and 2015 (9 wt. %) system targets

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