Study of Hydrogen Storage in Advanced Boron and Metal Loaded High Porosity Carbons Carried Out in the "DOE/NREL Center of Excellence on Carbon-based Hydrogen Storage Materials"

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5/23/2005

Project ID
STP#36

Overview

Timeline

- Project start date: FY05
- Project end date: FY09
- New Start

Budget

- Expected Total Funding
  - DOE Share: $1,200,000
  - PSU Share: $300,000
- Funding for FY05 for PSU: $50,000

Barriers

General:

A. Cost.
B. Weight and Volume.
C. Efficiency.
E. Refueling Time.

Reversible Solid-State Material:

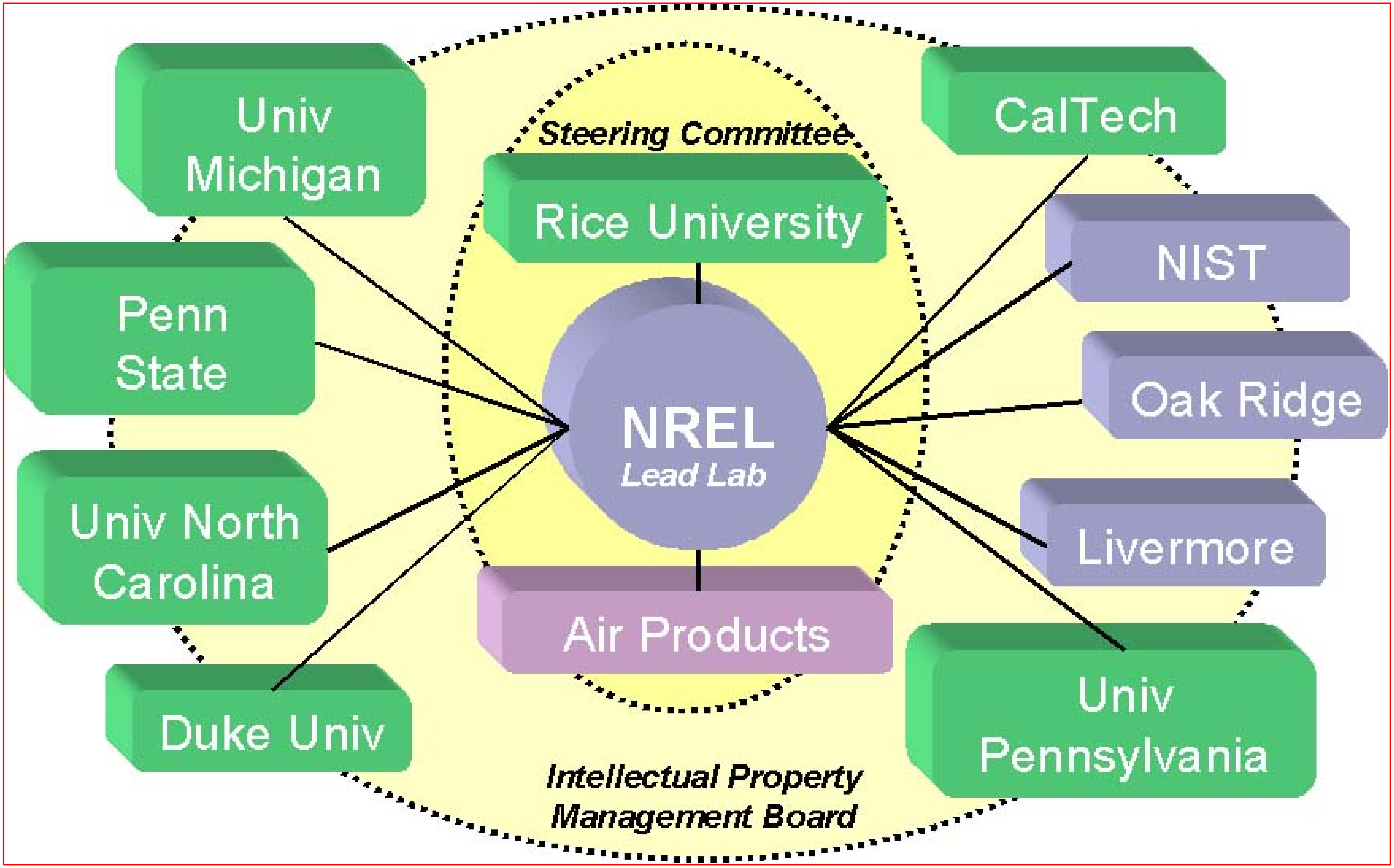
M. Hydrogen Capacity and Reversibility.
N. Lack of Understanding of H Physi- and Chemisorption.

Partners/Collaborations

We expect a highly complementary effort in all aspects of this work including materials synthesis and exchange, materials evaluation, sharing of structural and hydrogen sorption characterization techniques, as well as information exchange to further progress of the Center towards achieving DOE goals.

Overview

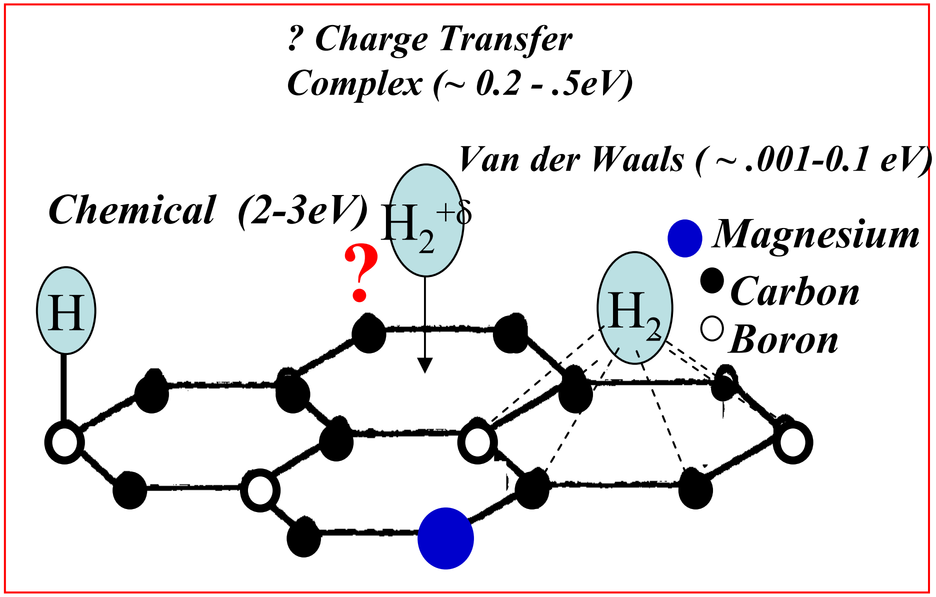
Partners/Collaborations



Motivation

Recent advances in the area of hydrogen storage in solid state materials have occurred that suggest that the discovery of new and better H-storage materials should be possible.

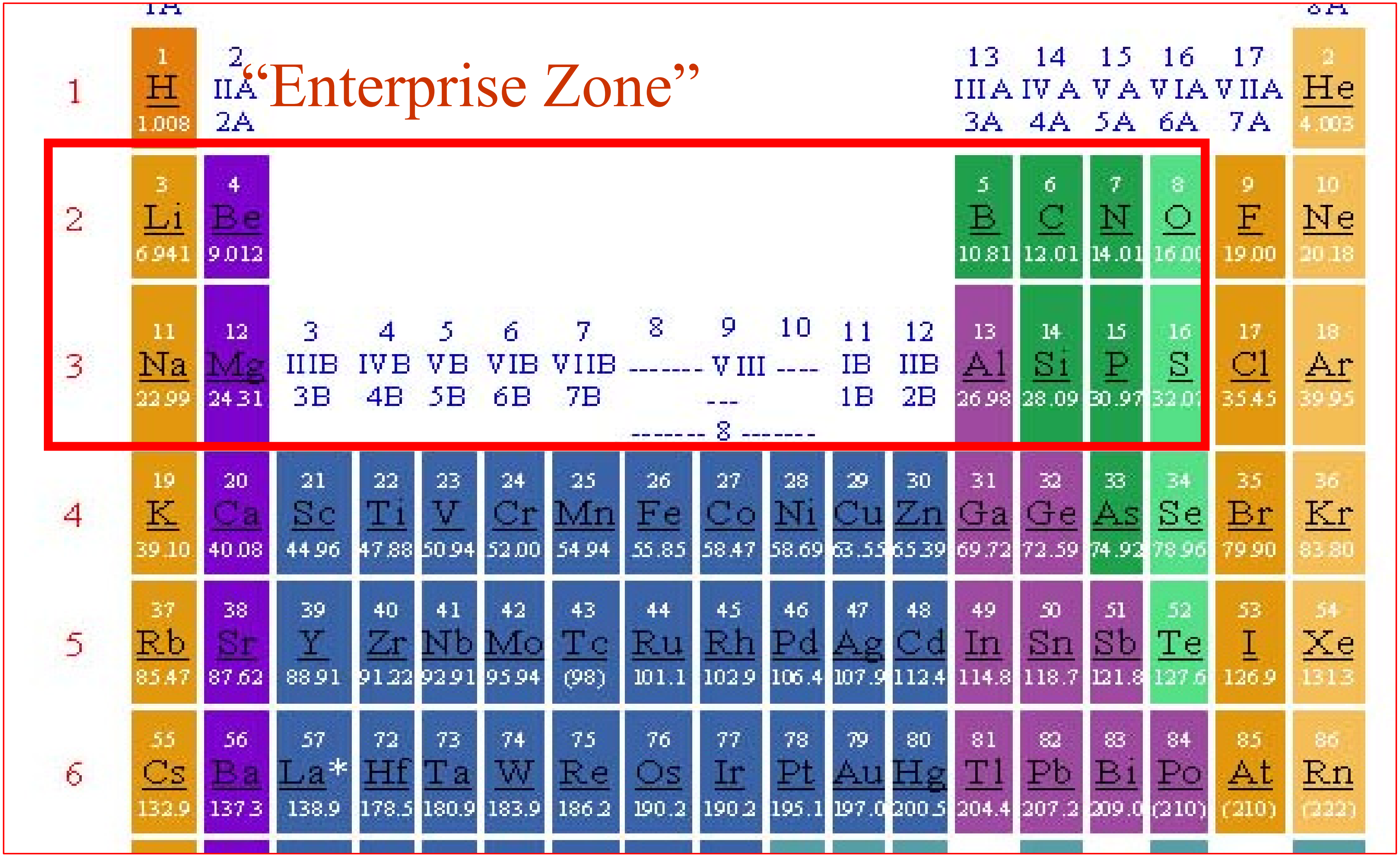
The gravimetric and volumetric storage of hydrogen in solid state systems is just now being shown to be sensitive to small adjustments in the bonding and structure of the host, and to the addition of small amounts of dopants. A better understanding of the nature of the metal-hydrogen bond and the influence of the chemical surroundings is emerging. New microporous cage materials have been discovered, whereby the pore openings allow transport of molecular hydrogen into the cages at elevated temperature.



Project Objectives

Develop and demonstrate reversible carbon-based hydrogen storage materials with at least 7 wt.% materials-based gravimetric capacity and 50 g H_2/L materials-based volumetric capacity, with potential to meet DOE 2010 system-level targets. Ternary high surface area materials are emphasized that are constructed from boron-doped carbon and light element metals. The relationships between the physical properties, H storage performance, pore size distribution and metallic character of the materials will be measured and connected with the local atomic chemistry and pore structure.

Project Objectives



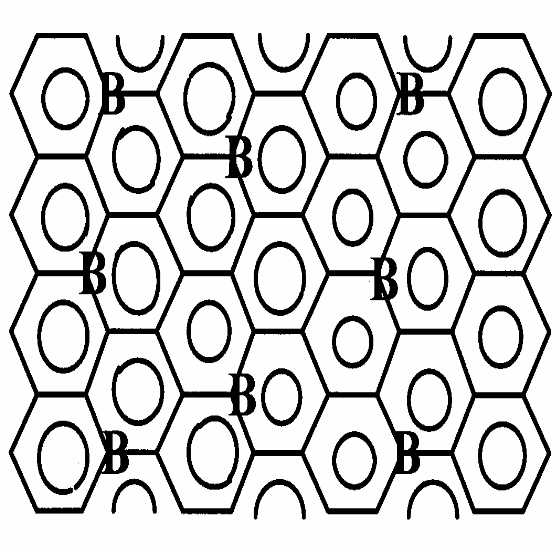
“Enterprise Zone”

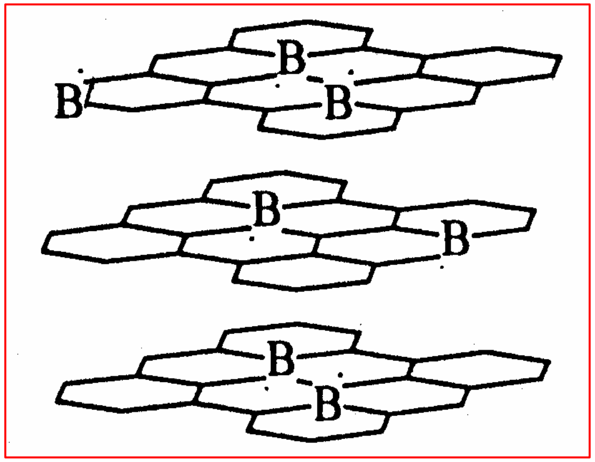
	IA	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8	9 VIII	10	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	8A
1	1 H 1.008																	2 He 4.003
2	3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.0	9 F 19.00	10 Ne 20.18
3	11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.0	17 Cl 35.45	18 Ar 39.95
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.47	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.59	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
5	37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
6	55 Cs 132.9	56 Ba 137.3	57 La* 138.9	72 Hf 178.5	73 Ta 180.9	74 W 183.9	75 Re 186.2	76 Os 190.2	77 Ir 190.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.5	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (210)	85 At (210)	86 Rn (222)

Approach

- Synthesis of C-B-M Materials
  - Pyrolysis of Molecular Precursor *(Professor Mike Chung)*
  - Inclusion Reactions with Preformed High SSA Carbons *(Professor Henry Foley)*
  - Very High Temperature Gas Phase Synthesis *(Professor Peter Eklund)*
- Synthesis of highly micoporous C-B-M material by three separate routes.
- Characterization of the short- and long-range structure, the microporosity and SSA
- Evaluation of these materials for hydrogen sorption behavior.
- Optimization of the SSA for specific C-B-M materials of technological relevance

C/B Materials (B-substituted C)

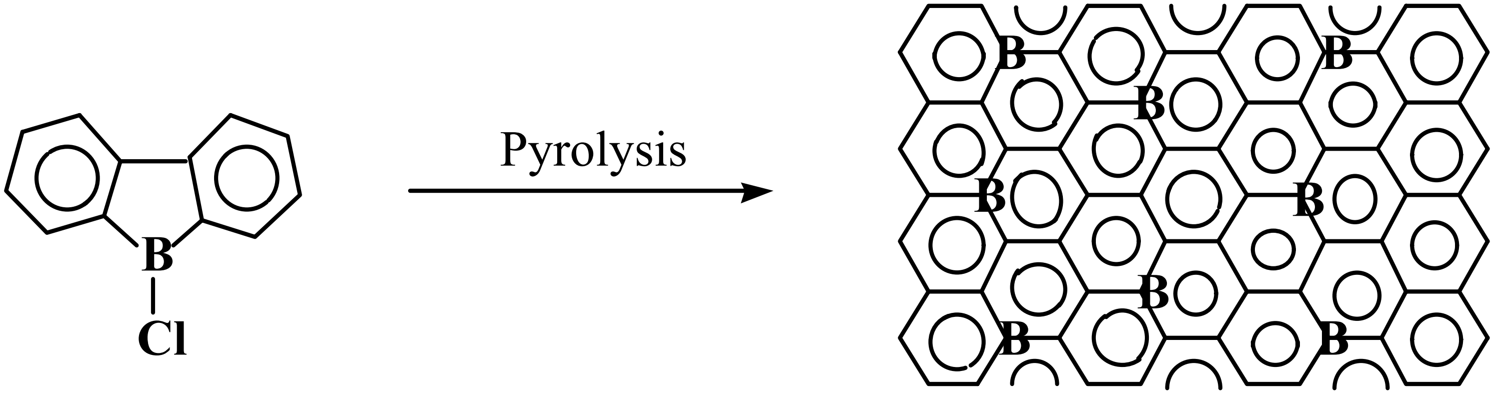




- C and B with similar atomic size with trivalent coordination,
  - C/B material can maintain graphitic structure.
- B (electron deficiency) serves as p-type dopant
  - Increase π-electron delocalization and surface activities.

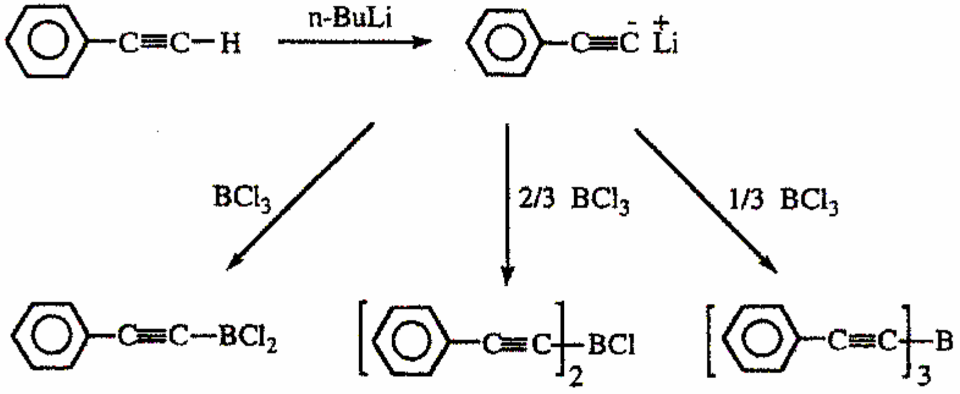
C/B Materials (B-substituted C)

Synthesis of C/B Materials by B-containing Precursors



CBF

B/C Material



DPB

BCB

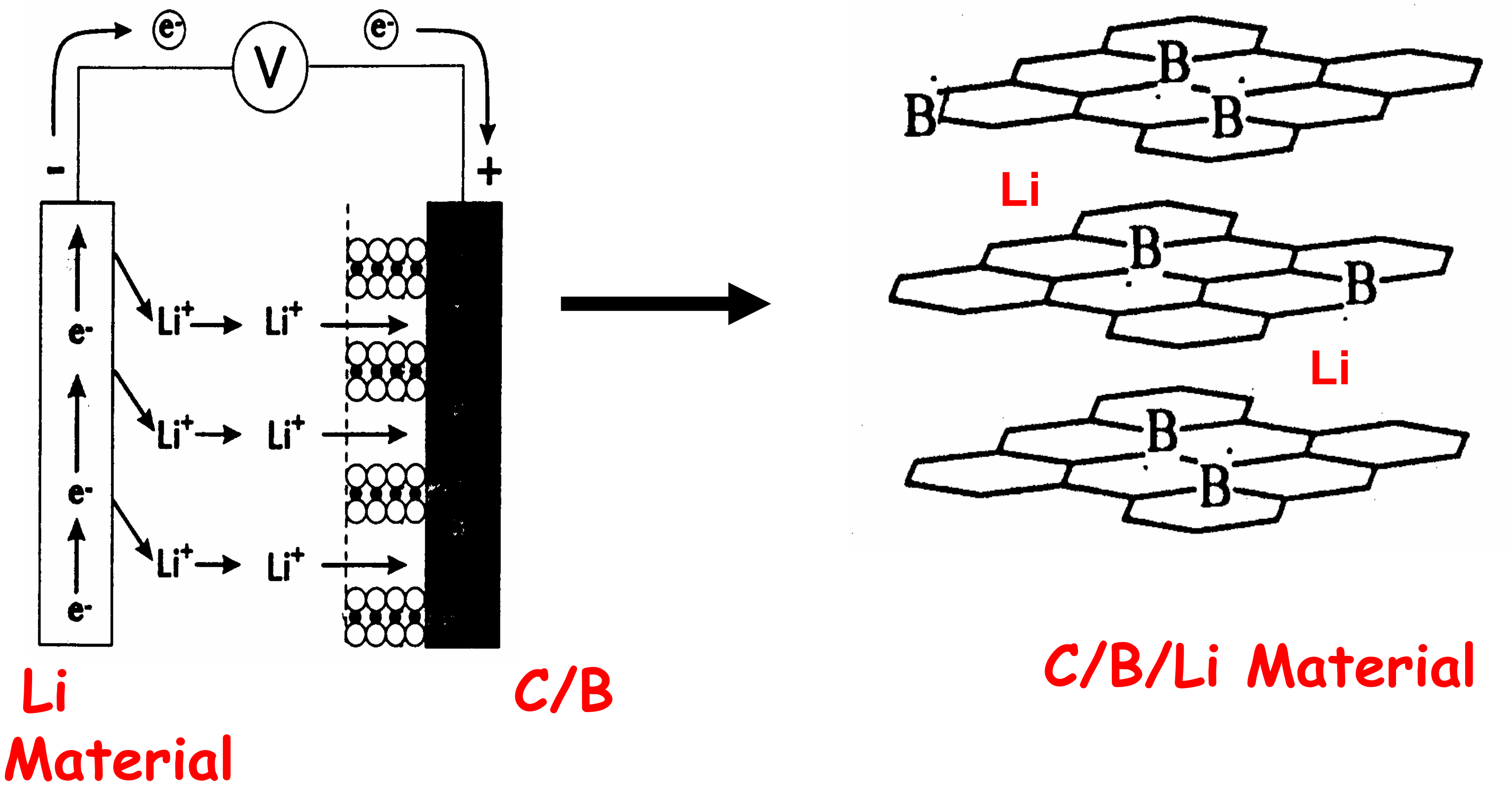
TPB

Equation 1

New C/B Precursors

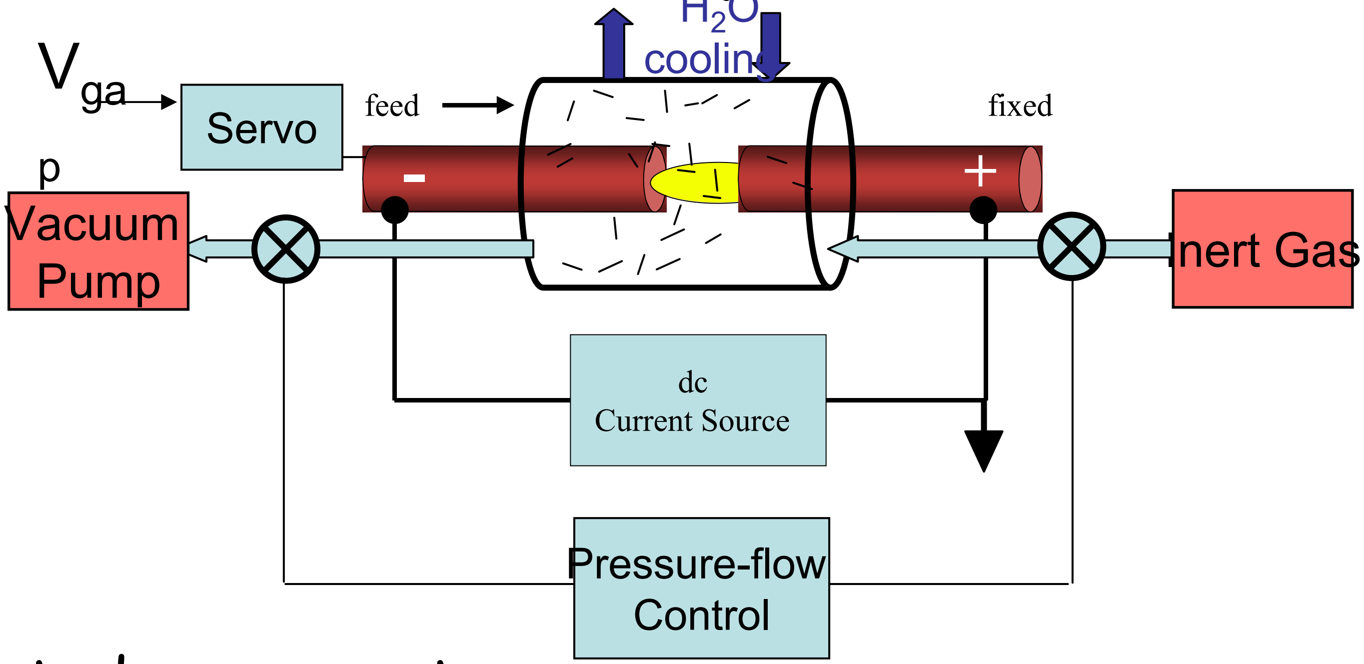
C/B Materials (B-substituted C)

Alkali-metal Doped C/B Materials



High SSA Carbons

Electric Arc Chamber for the Production

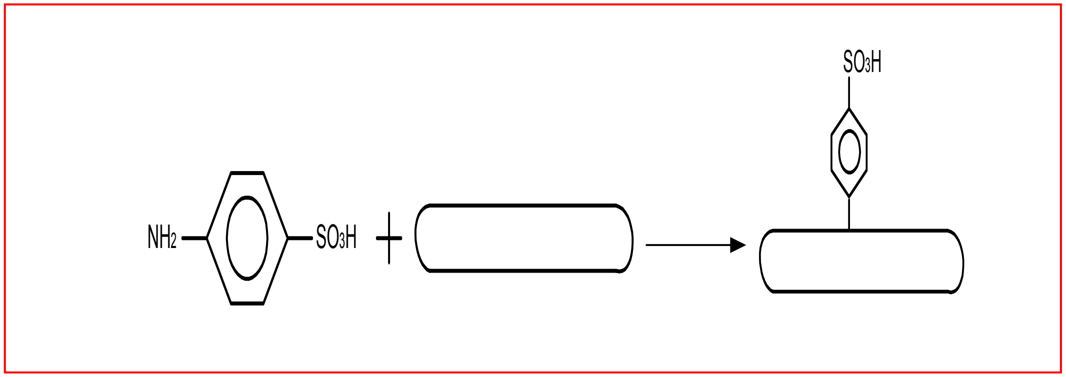


- Fully automated- no operator necessary
- 200 grams/day per chamber
- Five Chamber Facility will yield 1 kg/day
- Develop new nanoporous carbon and other lightweight nanomaterials synthesis (e.g.,BN nanotubes), *hybrid* "supported" nano-metal hydride materials

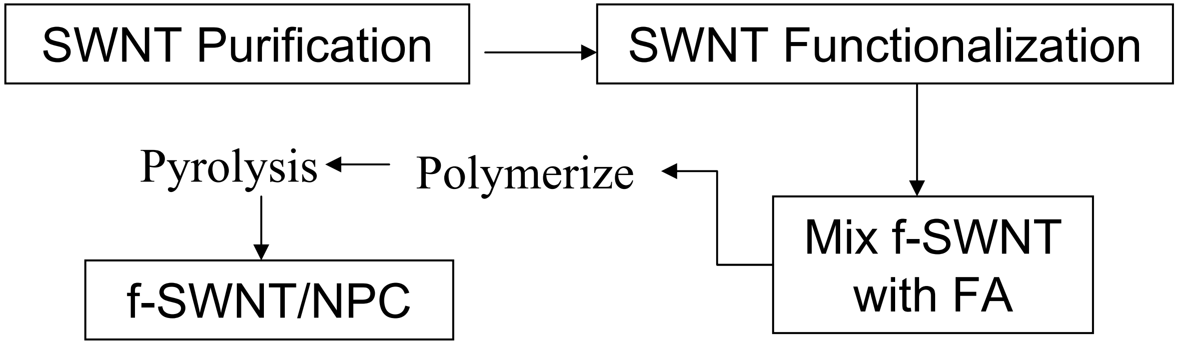
Nano-Porous Carbons

Modify Nano-Porous Carbons derived from PFA to increase the preferred adsorption sites for H_2

- Highly curved graphitic micro-domains in NPC
  - Active centers for adsorption and catalysis.
- Incorporate SWNT with NPC
  - May increase the curvature of carbon, which is helpful for adsorption.
  - Functionalization of SWNT is necessary for well dispersion of SWNT in NPC.



  - Process of preparing f-SWNT/NPC nanocomposites



SWNT Purification

SWNT Functionalization

Mix f-SWNT with FA

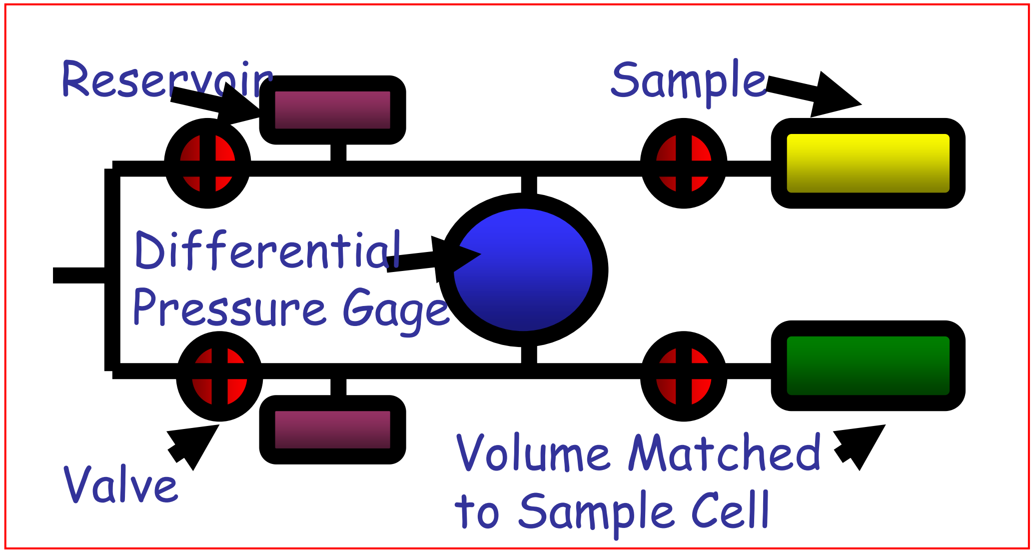
Polymerize

Pyrolysis

f-SWNT/NPC

Characterization

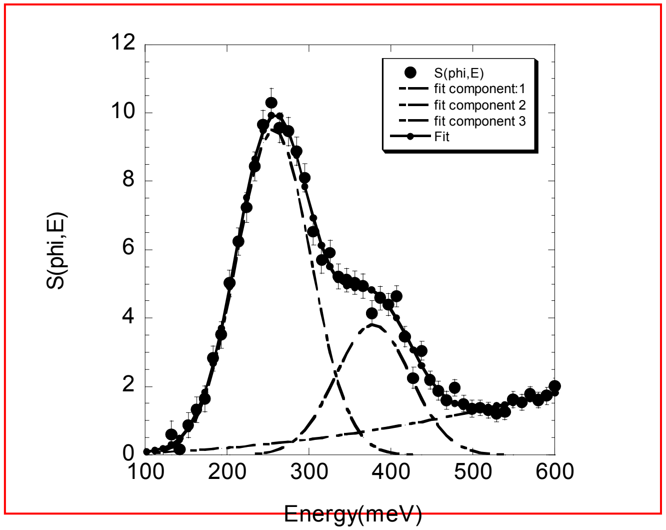
Hydrogen wt% Uptake



- High Precision Measurements of Hydrogen wt% with Differential Adsorption Apparatus
  - wt% uptake ∝ dP

Microscopic Dynamics of Adsorbed Hydrogen

- Microscopic Dynamics of Adsorbed Hydrogen Determined Through Neutron Scattering
  - Zero Point Energy
  - Self-Diffusion
  - Rotational Behavior
  - Ortho-to-para conversion



Future Plans

FY05

- Synthesis and hydrogen storage capacity study for at least one material made by each synthesis route described in poster. (4Q Year 1).
- Results of investigation of the possible benefits of additional spill over catalyst.

FY06

- Determine volumetric and gravimetric limits of performance of various porous C-B-M materials relative to 6 wt%, 4.5 gH_2/L system. (Go/No Go: 4Q Year 2).
- Determine optimal composition range and synthesis route.
- Determine effective H- binding energy for the most promising C-B-M materials

Future Plans

FY07

- Deliver at least one sample exhibiting H-storage performance characteristics that can meet FY10 system targets to DOE-specified facility (Go/No Go: 4Q Year 3).

FY08

- Scale up production of materials to the 100 gram/day range (4Q Year 4).

FY09

- Develop prototype 1 kg/day system (2Q Year 5).
- Deliver 1 kg active material that meets system goals (4Q Year 5).

Future Plans

Go/No-Go Decisions

- Determine volumetric and gravimetric limits of performance for C-B-M per unit SSA material relative to 6 wt%, 4.5 gH_2/L system (Go/No Go: 4Q Year 2).
- Deliver sample exhibiting material performance characteristics that can meet FY10 system targets to DOE-specified facility (Go/No Go: 4Q Year 3).

Hydrogen Safety

At PSU, safety is always a primary concern:

Services Offered:

- Laboratory Safety Inspections and Audits
- Laboratory Safety Training

Policies:

Compressed cylinders

- Must always be secured.
- Environmental, Health and Safety must do survey of area after release of H_2 into laboratory environment.

Safety plan specific to this project is under development