Overview of the DOE Hydrogen Sorption Center of Excellence

Anne C. Dillon, Director
Lin J. Simpson, Deputy Director
National Renewable Energy Laboratory
May 21, 2009

ST_22_Dillon

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Overview

Barriers Addressed

- Cost.
- Weight and volume.
- Efficiency.
- Refueling time.
- Hydrogen capacity and reversibility.
- Understanding of physi- and chemisorption.
- Test protocols and evaluation facilities.

Timeline

Start date:	FY2005
End date:	FY2010
Percent complete:	80%

Budget

Center Management - $380K

Partners: 9 universities, 5 government labs, 1 company

Steering Committee Members: APCI, Caltech, NIST, NREL, UM

Also, many other interactions with independent projects (BES and EERE), the other CoEs, IPHE, IEA, and companies…. see back-up slides for details.

Approach: Objectives and Center Management

Center Management:

- **Center assembles and coordinates a diverse group of experts**
  - From universities, government labs, and industry (see backup slides) with unique and complementary skill sets to achieve technical objectives
  - Partners organized in focused research clusters (RC) to optimize development and avoid duplication of effort, with seamless integration of experiment/theory
- **Continually monitors progress via steering committee and RC's**
  - Adjust technical direction to ensure efficient resource utilization to accelerates progress
  - Use quantitative down-select criteria prior to beginning R&D at go/no-go points

Center Objectives:

- **Develop Sorbent materials that will meet DOE 2015 system targets:**
  - High-capacity that operate at **modest pressures (e.g. less than 100 bar)** and below fuel cell operating temperatures **(<70C**).
    - Must substantially improve storage compared to compressed or cryocompressed tanks
  - **High surface area and high density**
    - Meet both gravimetric and volumetric targets simultaneously with rapid kinetics.
  - **Optimize binding energies via structure or electronic mechanisms**
    - Enables efficiently and rapid on-board refueling with minimum energy requirements
  - Devise facile synthetic routes using low cost approaches.

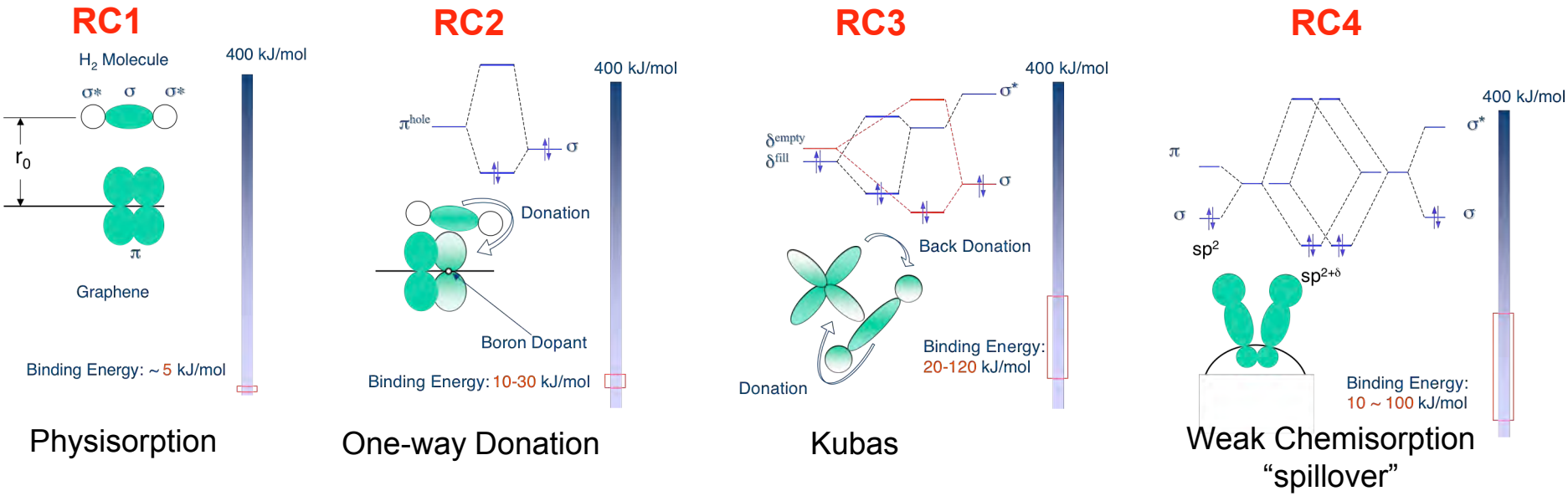
Approach: Research Clusters (RCs): Sorption Mechanisms

Organized focused teams based on sorption mechanisms

- **Accelerates efficient developments and ensures appropriate resources are available**
- **Enables tractable focused accelerated discovery and higher throughput**

Research Clusters

- **RC1: Engineered Nanospaces: optimize material density and surface area**
- **RC2: Substituted Materials: e.g. BC_3 to enhance binding energy**
- **RC3: Strong Binding: stronger interaction with atomic metal atoms**
- **RC4: Spillover: catalytic dissociative adsorption**
- **Theory coordinated across RCs, design materials & synthesis (see back up slides)**



- **RCs complimentary, building on each other to make an optimized material:** e.g. molecules developed in RC3 can be localized on doped (RC2) high surface area (RC1) materials.

- **All RCs balance hydrogen and material reactivity with the density and stability of the sorption sites. Materials being developed to operate from ~100 to 350K at moderate pressures with no significant thermal management issues to efficiently meet DOE targets.**

Approach: Relevance to DOE

- **Typically, sorbents meet 13 of 16 DOE storage targets**
  - **Paths available to meet 2015 and perhaps ultimate targets**
  - Potentially require least engineering to meet HSECoE Phase I and II goals

Storage Parameter	Units	2010	2015	Ultimate
System net Gravimetric [a]	kg H_2/kg system	0.045	0.055	0.075
System Net Volumetric	kg H_2/L system	0.028	0.040	0.070
Storage system cost [b]	\$/kg H_2	133	67	TBD
Durability/Operability 1. Operating ambient T [d] 2. Min/max delivery T 3. Cycle life (1/4 tank to full) [e] 4. Cycle life variation [f] 5. Min del. P from storage 6. Max del. P from storage [g]	°C °C Cycles % mean (min) at % confidence Atm (abs) Atm (abs)	-30/50 (sun) -40/85 1000 90/90 4FC/35 ICE 100	-40/60 (sun) -40/85 1500 99/90 3FC/35 ICE 100	-40/60 (sun) -40/85 1500 99/90 3FC/35 ICE 100
Charge/discharge Rates • System fill time (5-kg H_2) • Minimum full flow rate • Start time to full flow (20ºC) [h] • S t art time to full flow (-20ºC) [h] • T . Resp. 10%-90%, 90%-0% [i]	min (Kg H_2/min) (g/s)/kW s s s	4.2 min (1.2 kg/min) 0.02 5 15 0.75	3.3 min (1.5 kg/min) 0.02 5 15 0.75	2.5 min (2.0 kg/min) 0.02 5 15 0.75
Fuel Purity (H_2 storage) [j]	% H_2	99.99 (dry basis)		
Env. Health & Safety • Permeation & leakage [k] • Toxicity • Safety	Scc/h - -	Meets or exceeds applicable standards		
• L oss of useable H_2 [l]	(g/h)/kg H_2 stored	0.1	0.05	0.05

*The storage system costs are currently under review and will be changed at a future date

Green: low risk, high probability to meet.

Yellow: medium risk, medium probability to meet.

Red: High risk, low probability to meet.

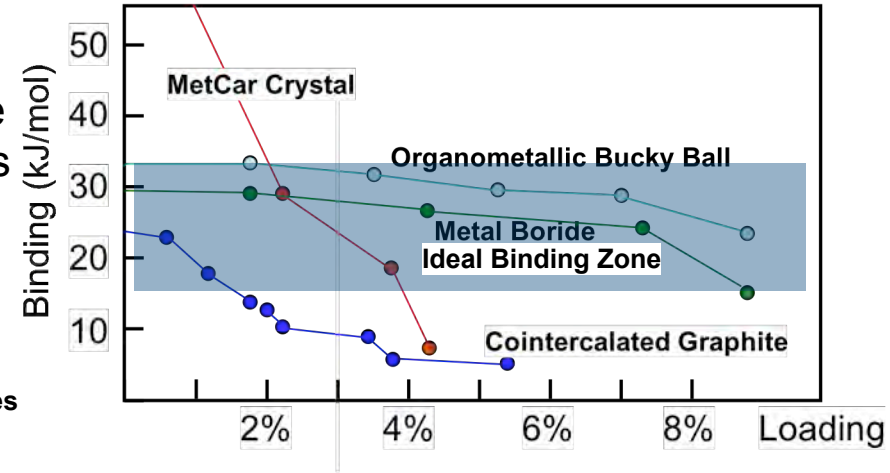
Depending on the exact sorption mechanisms and materials used, **only cost and capacity are typically an issue for sorbents**.

- Most HSCoE efforts focused on these 3
- HSCoE may have several materials that will meet DOE 2010 system targets
- HSCoE may have materials that meet HSECoE phase II goals
- HSCoE works to meet ultimate targets

Approach: Binding Energy, Coverage, Gravimetric, Volumetric

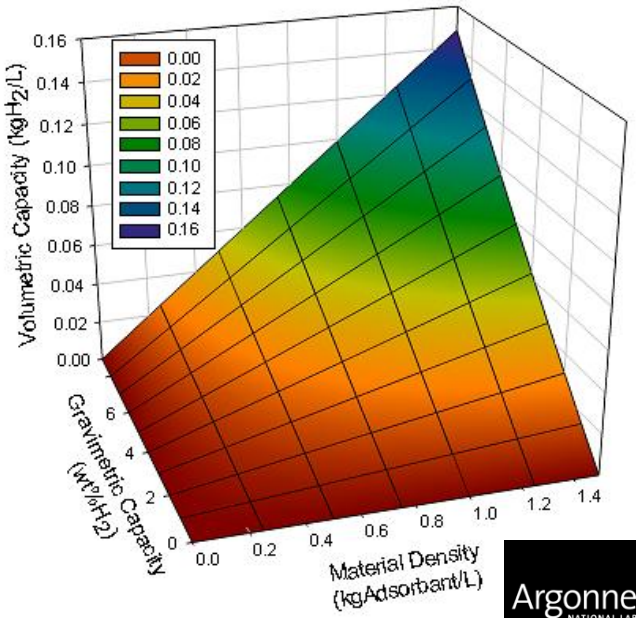
H_2 binding & site access affect capacities

- For physisorption binding decreases w/ coverage
- For more complex structures unique binding sites saturate in order of binding energy
- **Goal: create nanostructures where ideal binding accessible for most of the capacity**
  - Decrease engineering design problems
    - **e.g. minimizes operational temperature and pressure ranges**



Higher density high SSA materials solves DOE volumetric challenges

- Increase volumetric capacity and gravimetric capacity simultaneously by increasing both specific surface area and packing density
  - Optimize uniform pore size between 0.5 to 1 nm
- Volumetric capacity is proportional to both gravimetric capacity and *material density*
  - **Materials densities typically 0.2 to 2 g/ml**
    - e.g. ANL Optimized pore size material with **~2000 m^2/g material with 1.4 g/ml density**
      - **LH2 densities (70 g/L) exceeded even with 5 wt% material**

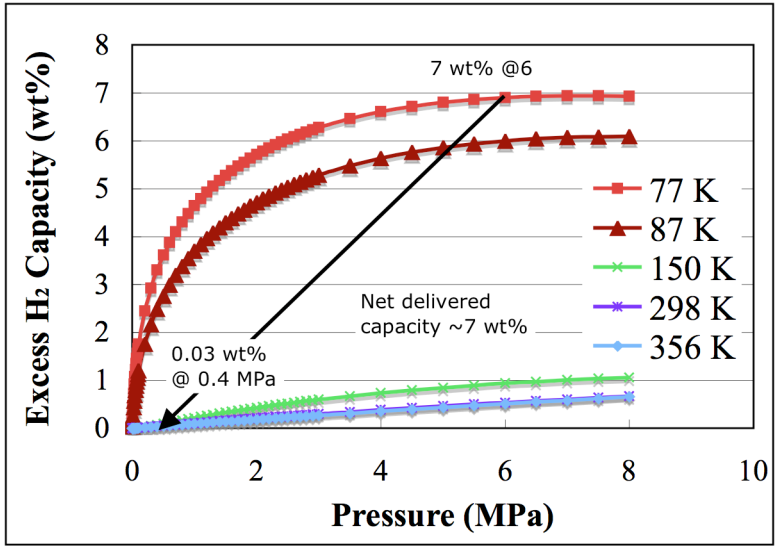


HSCoE develops structures with a high number of sites with enhanced enthalpies of adsorption that persist to high coverage. Optimized pore sizes can greatly improve volumetric capacities to help meet DOE targets.

Accomplishments Overview: Access to Optimized Sites

Previous Accomplishments

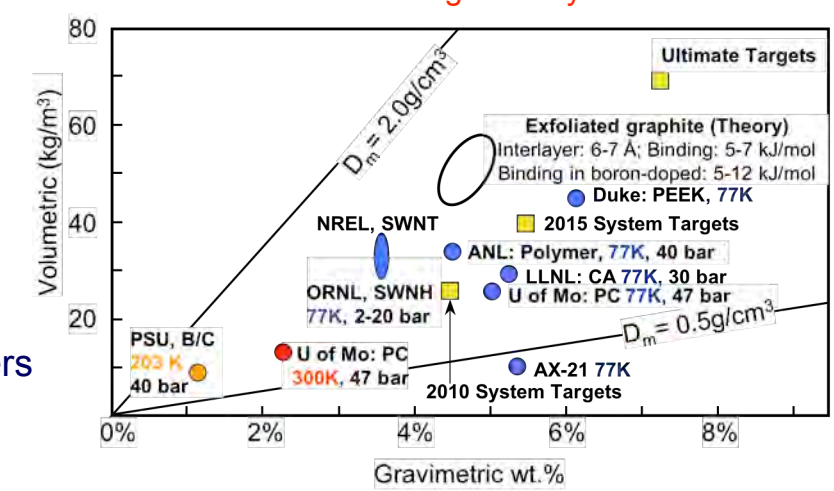
- For high SSA sorbents focus on cost and capacity
  - > 7 wt% material capacities demonstrated
  - May be **closest to 2010 targets** to meet HSECoE goals
  - **No significant heat transport issues**: see back-up slides
  - Lower pressure and higher temperature reduce costs
  - Surface/H_2 interaction (i.e. enthalpy) changes binding



Dubinin-Astakhov Model Fit of MOF-177. >95% of stored H_2 will be delivered at 4 bar or higher. Tank heats from 80 to 300 K during delivery.

Accomplishments since last AMR

- **>95% of material capacity delivered from tank**
  - 80 to 300K and 50 to 4 bar transitions
- Synthesized new high SSA materials with optimized uniform pore size; scalable/inexpensive processes
  - **Templating:** enables exact materials and structures
    - Duke: PEEK, >6 wt% with ~0.8 nm pore size
    - NREL: Zeolites, ~7 wt% demonstrated
  - **Graphene:** high conductivity and durability
    - Rice: Exfoliated Graphite, CNT scaffolds
    - NREL: co-intercalated graphite
    - **Caltech: uniform higher binding for all loading**
  - **Aerogels:** LLNL: scaffolding
  - **Chemical or Vapor** Synthesis
    - TA&M-MOFs, ORNL-SWNH, Rice, NREL, ANL-polymers
      - **TA&M created materials with 9000 m^2/g**
      - **ANL: 1.4 g/ml material with ~2000 m^2/g**
  - **Pyrolization:** Missouri-corncobs



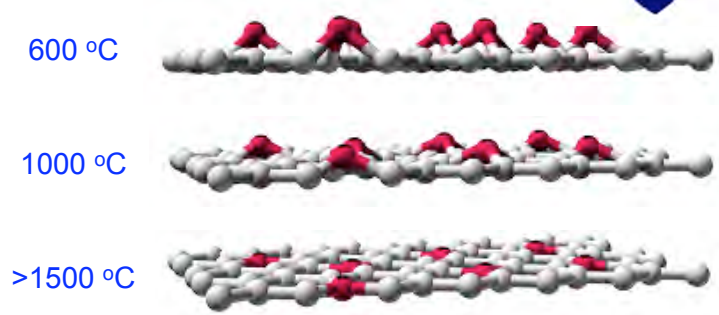
Developed multiple new materials that may meet the 2010 DOE vehicular hydrogen storage system targets including cost, gravimetric and volumetric.

Accomplishment Overview: Substitution Improves Storage

PENNSTATE

Previous Accomplishments

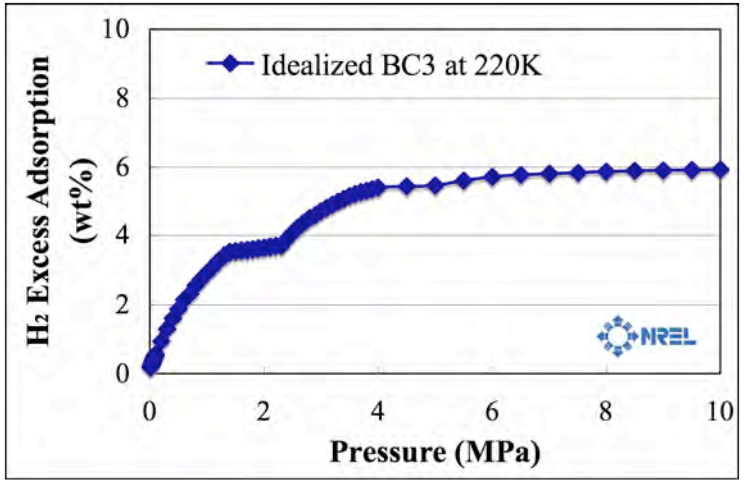
- HSCoE pioneered substituted materials for hydrogen storage
  - Electronically "frustrated" B in graphene binds H_2 at ~11 KJ/mol
    - e.g. Kim et. al. PRL 96, 016102 (2006)
  - **Calculations confirmed by experimental measurements**
    - e.g. Chung et.al. JACS Comm. (2008), PSU & APCI AMR 2009
    - Experiment and theory loop closed!
    - Besides Be, other elements in carbon have little impact
    - Other C-B bonding configurations have little impact
    - Investigated other materials systems, e.g. F: APCI
- High SSA B-C materials improve capacity and increase storage T's.
  - Reduce system costs by increasing the cooled storage temperature and/or lowering required pressure



Puckered structure of appropriate boron substituted C is required for higher binding energy.

Accomplishments since last AMR

- **>5 wt% delivered capacities achievable at -50°C**
  - For ideal material with access to every B in BC_3, @~100 bar
  - Value increases with lower storage temperature
  - Highly impact volumetric capacity at near ambient
- Investigated three main methods to synthesize B-C materials with high surface area using scalable/inexpensive processes
  - Create high surface area with high B content precursors
    - PSU: pyrolisis of BC_2-X; higher B with high SSA
  - Template BC_3: NREL, Zeolites & AC; Duke, PEEK; APCI, theory
  - Replacement: Missouri-corncobs
- Still have issues with higher B only with lower SSA
  - Best so far is ~12% B and ~800 m^2/g
  - **Must balance processing conditions to optimize SSA and B**
  - **BCx helps bind metals and improves spillover**



Idealized porous BC_3 could deliver >5 wt% H_2 (>50 g/L) at -50°C.

Designed/developed substituted materials to enable higher hydrogen binding energies in porous materials. Demonstrated higher B concentration (10-15%) in carbon with higher surface area (800 m^2/g). BCx could increase the storage tank temperature and capacity, thus reducing overall system costs.

Accomplishments Overview: Multiple H_2 Binding by Metal Centers

Previous Results:

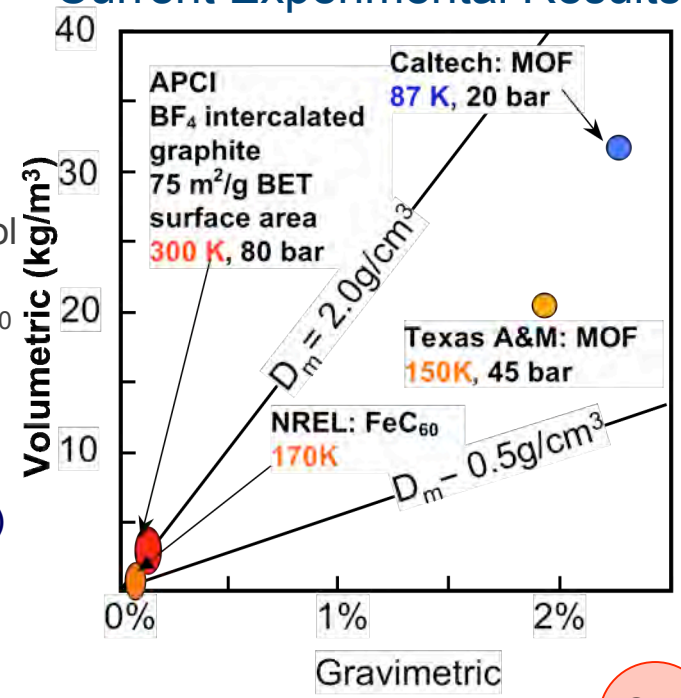
- Zhao et. al. (2005) pioneered new H_2 storage materials
  - Initial calculations calibrated by accurately predicting experimentally measured Cp-M, C-M, and X-M-H_2 binding
    - **Predicts # and binding of all known 3d M-H_2 samples**
    - e.g. H_2-Mn-MOF: experiment 10 kJ/mol, theory 8.4 kJ/mol
      - Sun, Kim, Zhang, JACS129, 12606 (2007)
      - Binding mechanism is same as metal decorated C_{60}

Accomplishments since last AMR

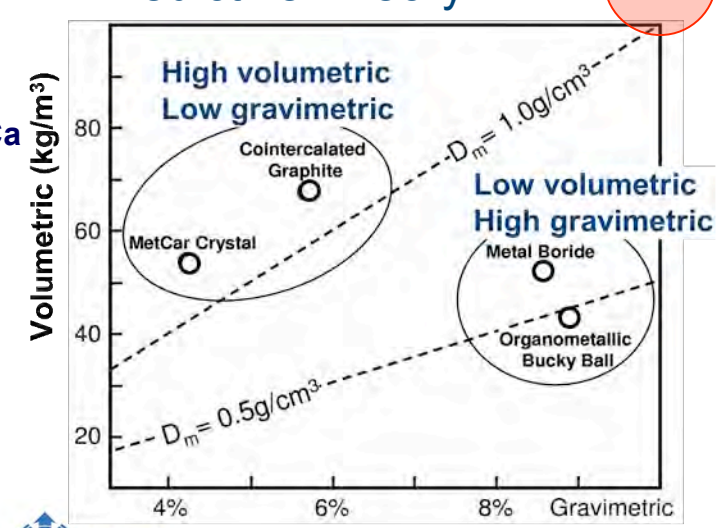
- Investigated multiple methods to form coordinated but e-unsaturated single metal structures binding >10 kJ/mol
  - Ti-silanol: ~2.7 H_2 -Ti @ ~22 kJ/mol-H_2 (Hamaed, JACS 2008)
    - NREL/RPI theory 2.4 H_2 stored/Ti @ ~30 kJ/Mol-H_2
    - **Validates metal decorated C_{60} predictions**
  - Metal decoration on high surface area materials
    - ORNL: Ca decorated SWNHs;
    - APCI: BF_4 intercalated graphite
    - TA&M: Open metal centers in MOFs
    - NREL: TM atoms with functional groups and BCx
      - Down selected some chemical synthesis routes
      - **Unique stability and multiple H_2 storage properties of Ca**
      - **>10 wt% & >100 g/L > liq. H_2 density but at ambient Ts**

Developed new materials with stronger H_2 binding either through interactions with exposed metal centers or electrostatic effects. This work paves the way to meet DOE's ultimate storage targets with RT storage densities >LH_2.

Current Experimental Results



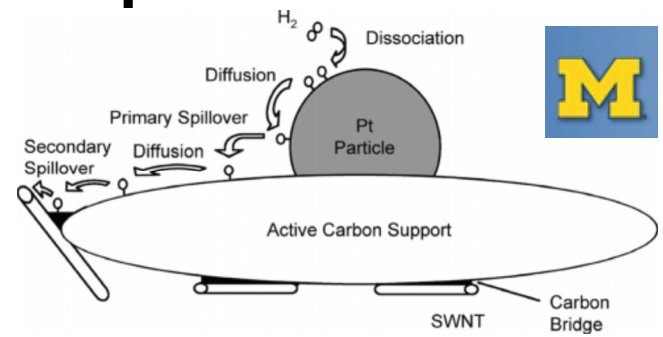
Predictive Theory

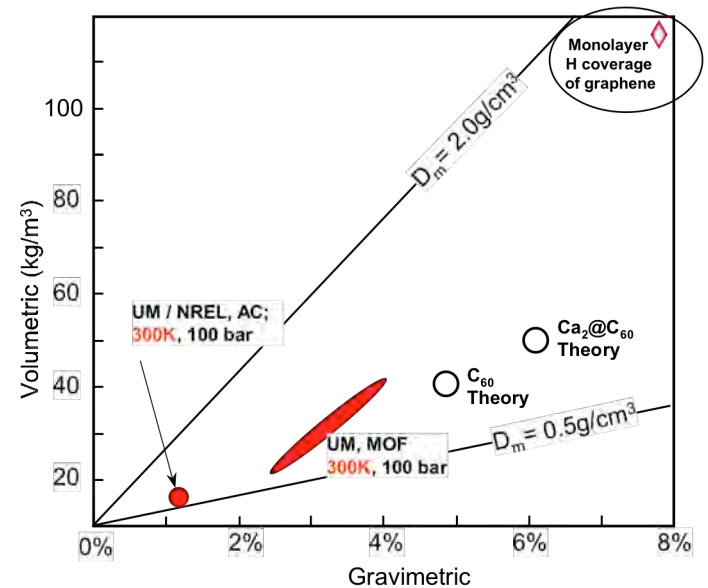


Accomplishments Overview: Improved Spillover Materials

Previous Results

- **Spillover effects observed on numerous materials**
  - Carbon 1.6 wt%, Pt/AC bridged MOF 4 wt% @ RT
    - No other MOFs tried have as high a capacity
      - e.g. COF-1, HKUST-1, MIL-101, MOF-177 (Yang 2008 AMR)
  - **10-20 KJ/mol binding energies measured**
  - **Dissociation observed with D_2/H_2 experiments**
  - **C-H spillover binding observed; neutron and IR**
  - **Desorption rates meet DOE H_2 delivery rate targets**
- Calculations confirm experimental observations
  - Indicate 7-8 wt% (50-60 g/L) capacity at RT
    - 7.5 wt% hydrogenation demonstrated
  - **H configurations identified that have observed energies**
    - **Main issue is how H moves along lattice (kinetics)**





Accomplishments since last AMR

- Functional groups affect hydrogen uptake
  - UM: oxygen, CH_4 increase uptake >15%
    - TiCl and VCl increased sorption rates
  - **NREL: smaller better connected catalysts increase uptake/rate**
    - **Fueling rate targets may be met with ~80% fill at 100 bar**
- Robust reproducible synthesis still major issue
  - UM, NREL, Caltech/LLNL, ORNL
    - Inconsistent results batch to batch and lab to lab

SSWAG analysis: ~3 wt% H storage if IRMOF 4 wt% spillover material used.

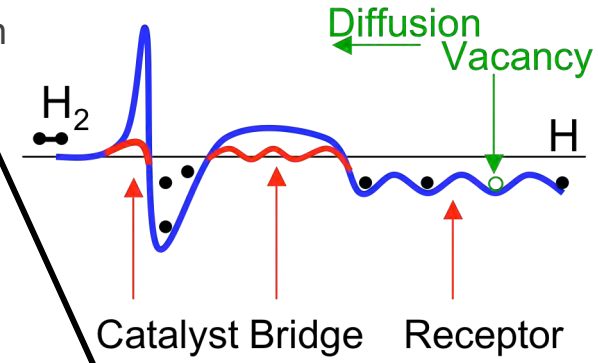
• ~8wt% spillover material could meet the DOE 5.5 wt% and 40 g/L 2015 hydrogen storage targets.

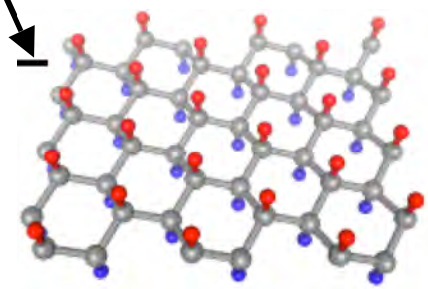
Identified new material processes that increase sorption rates and hydrogen storage capacity by > 15% at room temperature.

Accomplishments Overview: Understanding Spillover

Previous Calculations Confirmed Experimental Observations

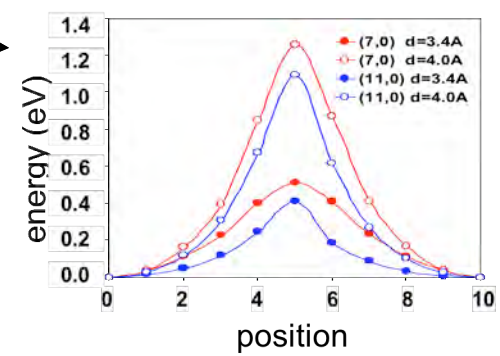
- Rice: First principles models identified H nucleation as a viable phase with ~20 KJ/mol effective binding energies
  - Energies for migration via H vacancy too high and H on both sides required
- APCI: Calibrated models with MoO_3 system, propose H physisorption as transport mechanism
- NREL: Previously developed models for hydrogenating endohedral fullerenes and metcars are applicable
- **Consensus that thermodynamics are allowed**
- Prehydrogenation of the receptors may be required





Improved Modeling Accomplishments since last AMR

- **NREL identified for 1st time potential structural & electronic mechanisms that enable H transport on sorbent surfaces**
  - H migration in nanoscale carbon materials mediated by a neighboring surface that approaches to ~3.4 Å
    - i.e. **hopping between surfaces faster than diffusion on surface**
  - NREL/RPI: **Holes** in valence band (e.g. doping or defects) lowers energetics and enables H transport
  - **Improve with optimal structures and doped/functionalized materials**
- **APCI: BC_3 catalyze H_2 dissociation and spillover migration**
  - Study kinetics and alternative less expensive spillover catalyst
- **Rice: Study metal saturation and catalyst-receptor transport**



Improved spillover kinetics understanding enables materials to be designed with higher capacities and sorption rates that can meet DOE 2015 targets. Identification of hole induced improvements along with receptor catalytic properties points toward inexpensive spillover material with fast sorption.

Example Collaboration RC4 (Spillover)

Motivation: Enhance Room Temperature H spillover

H theory
NREL/RPI-Kinetics, UM
Rice, APCI-thermodynamics and catalyst

Materials Synthesis

Spillover materials:
Catalyst-Carbon (NREL, LLNL, ORNL,)
MOF and others (UM, NREL)

Measurement & Characterization

Small volumetric & TPD - NREL

Prompt Gamma
NIST

High Accuracy
Volumetric - APCI

NMR - UNC

Volumetric - UM

Progress?

yes

no

Clusters focus and accelerate efforts to, e.g., synthesize materials with higher spillover capacity and rates, for improved hydrogen storage.

HSCoE Coordination, Collaborations and Communications

- Center has > **42** joint projects and > **30** joint publications: e.g.
  - **Focused RCs create collaborations** among HSCoE partners (see slide 5)
    - Each RC is co-led by NREL staff and a steering committee member
    - Effectively leverages unique partner capabilities to accelerated materials development while closely coordinating activities to minimize duplication
    - Enables focused coordination to maximize advanced materials development
  - See partner presentations for specific collaborations
  - **Theory is actively coordinated** by steering committee and theory group to ensure efforts work closely with experiment to foster the best interactions that maximize materials development
- HSCoE **actively coordinates resources to maximize progress** and overall funding through formal program evaluations (internal and with TT and AMR reviewers), direct center wide or RC discussions, and informal small group interfacing for highly focused development

- **HSCoE actively manages unique partner capabilities and overall resources to accelerate hydrogen storage materials development.**
- **HSCoE has dozens of collaborative interactions that are openly discussed, evaluated, and redirected during face-to-face meetings and with web-casts either in small groups or by the whole center.**

Collaborations and Leadership Outside the Center

- **HSCoE partners work with > 43 groups around the world,** e.g.
  - LLNL works directly with MHCoE partners: put MH into carbon
  - Caltech & NIST part of **MHCoE** and and APCI in **CHCoE**
  - NIST performs neutron scattering for groups from around the world to determine hydrogen interactions and material properties
    - e.g. ISIS (U.K.), Monash U., U. Nottingham, Berkeley, GM, ORNL, U. Sydney,
  - NREL works with numerous groups outside HSCoE and is part of **HSECoE**
    - ANL and SSWAG on hydrogen storage system design and analysis
    - Lead efforts in hydrogen storage measurements and instrumentation
    - Work with groups to validate results: e.g. Stubos' group, Demokratos, Greece
- **Partners organize conferences around the world**
  - e.g. MRS, ECS, APS, ACS, (see partner presentations)
- Partners published **>90 papers** and gave **>112 presentations**
  - CoE members are reviewers for publications submitted to many journals
- See partner presentations for more examples and details

- **HSCoE works w/ dozens of groups & provides leadership throughout the world.**
- **HSCoE works closely with DOE, other storage centers, & BES/NSF/DoD projects.**
- **As seen by the huge surge in publications and technical conference participation HSCoE instrumental in accelerating hydrogen storage materials development.**

Down-Selects and Materials Recommendations

- **The HSCoE Steering Committee with DOE developed "Down-select Criteria" for the center materials**
  - Separate criteria were developed for each cluster (See backup slides)
    - Criteria considers material gravimetric, volumetric, rate and cost potentials
  - **The criteria will be employed for all Go/No-Go decisions**
    - All HSCoE material design and development work will meet criteria
  - A **document** with all center **down-selects** (currently 40) is continually **being updated** and will be provided as a deliverable in 2010
- **HSCoE materials development roadmaps for each RC**
  - Details work for rest of center and projects required efforts through 2015
- **Provide material recommendations to DOE and HSECoE**
  - 2010 provide DOE with **comprehensive report and publication** of HSCoE materials development efforts and recommendations for future activities
  - Based on **HSECoE** Phase I and Phase II criteria, provide material recommendations and performance characteristics
    - Enable HSECoE to select materials for further analysis and potential hydrogen storage demonstration systems

HSCoE actively evaluates and redirects efforts as needed to ensure optimum materials development and to help DOE manage it's portfolio

Examples of Down-selection, Redirection of Resources

LLNL (Baumann): RC1

- Improving undoped activated carbon aerogels work stopped
- Capacity < ~5.5 wt% & ~40g/L
- Focus on substituted materials and using aerogels at scaffolds

To date 6 material classes down-selected

NREL (Engtrakul): RC3

- Chemical synthesis work stopped on Co or Fe:C_{60} & Sc-aminobenzyl
- New directions focus on known routes to stabilizing metal atoms on solid supports using BCx materials

To date 15 material classes down-selected

APCI (Cooper): RC2

- Li doped SWNT's discontinued due to small observed capacity
- Investigate F and BF containing compounds that may provide enhanced binding

To date 3 material classes down-selected

Spillover (Yang, *et al.*): RC4

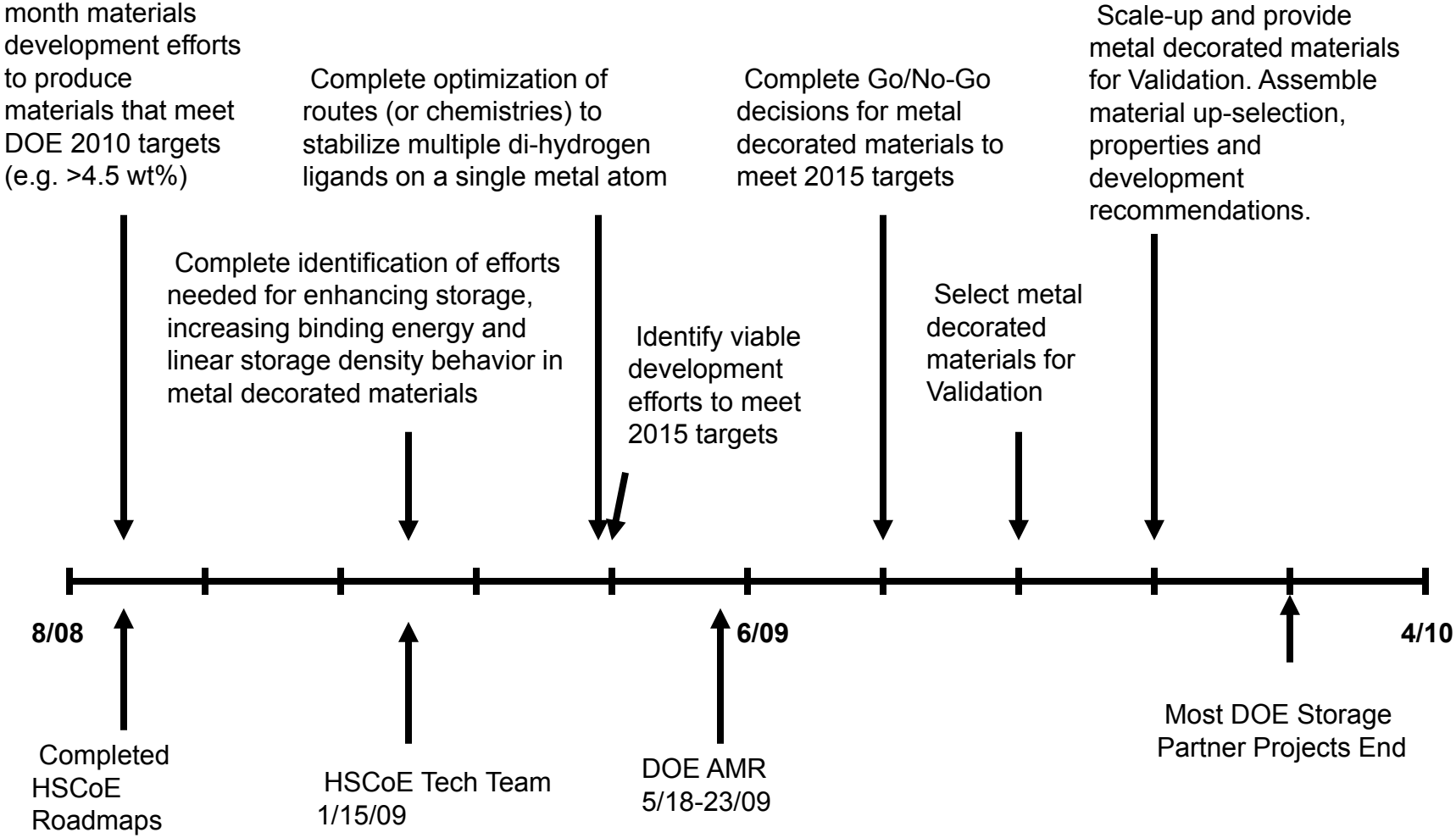
- Work on Pd-doped MOF-177 stopped due to low capacities
- Concentrating on reproducibility of processing, kinetics, increasing capacities, etc.

To date 16 material classes down-selected

Example **Roadmap**: RC3 Strong Binding Timeline to 2010

- Roadmaps have been developed with input from Partners, DOE, and the Tech Team, and bring structure and quantitative short and long -term goals to the RC-level
  - Roadmaps contain detailed objectives, individual partner development efforts, go/no-go decisions, and timelines for directed work to be done through 2010 and 2015.

Example of RC3 Timeline in roadmap for work through 2010



HSCoE FY09 and FY10 Efforts

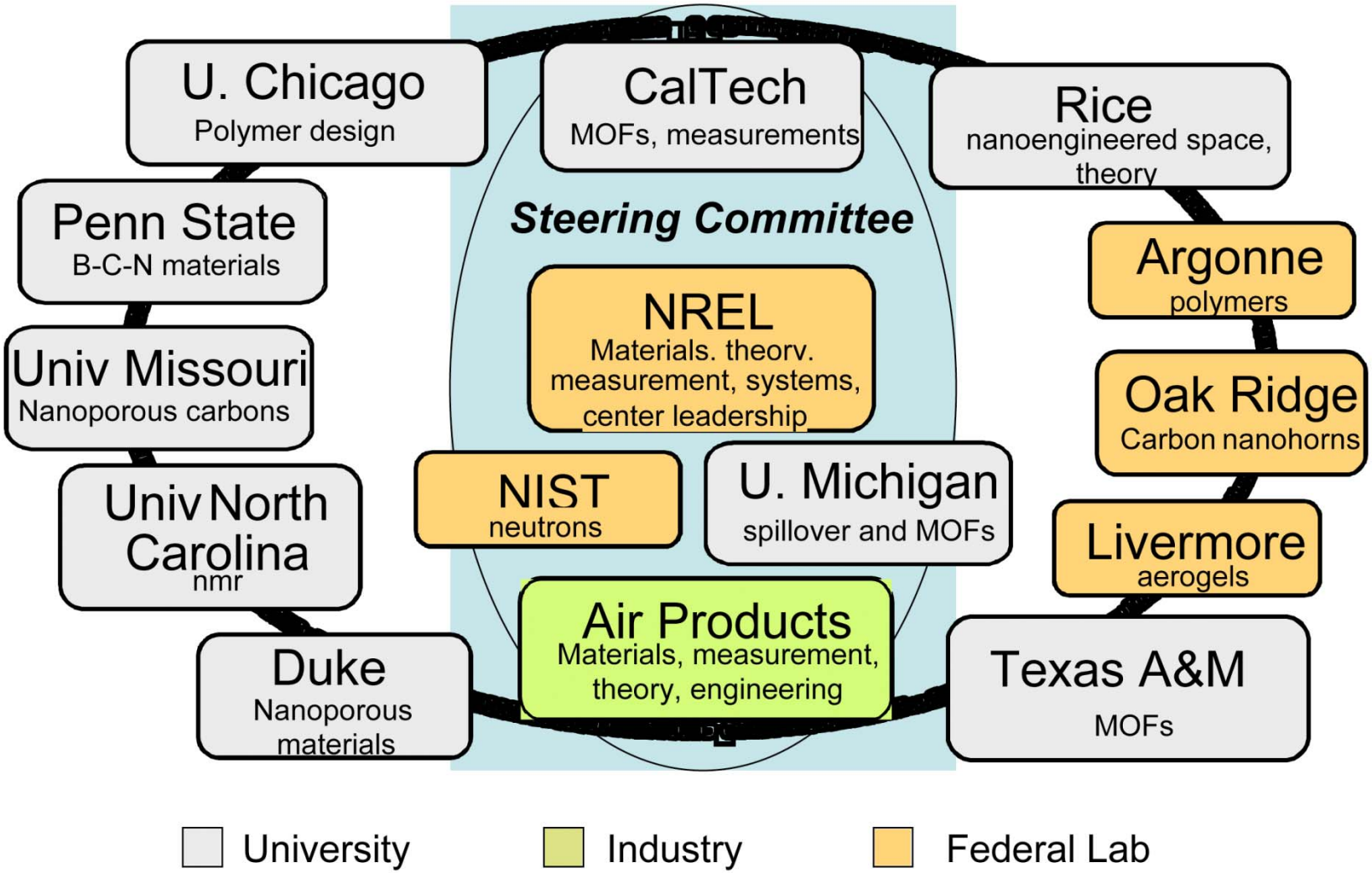
- **Clusters:** Wrap up focused materials development work and complete materials characterization and validation. Maintain awareness of advances made in different clusters and other groups, and insure efficient coordination of efforts.
  - **Porous materials:** Develop high surface area materials with optimized pore structure for efficient volumetric capacities and enhanced hydrogen binding. Integrate substituted elements (e.g. boron in porous carbons) produced by, scalable processing (eg., templates, propped graphenes, carbon and non-carbon aeroges). Work interactively to characterize the structure properties, analyze the optimal pore effect, and investigate the highest potential for H storage for different sorption mechanisms. Leverage carbon-based material experience to determine if other light elements can be used to implement mechanisms more straightforwardly, or if brand new, more desirable approaches may be found.
    - **MOF Materials:** Further enhance H2-MOF interactions by preparing materials with a higher density of coordinatively unsaturated metal centers, improve H2 uptake at temperatures higher than 77 K by ligand and MOF design, increase MOF thermal stability while maintain its porosity. Increase volumetric performance using denser H2 packing and optimal pore sizes.
  - **Metal decorated structures:** Focus on tractable processing with identification of atomic structures, characterize the reactions, simulate their H-storage properties, and improve the properties.
  - **Spillover Materials:** Work in well coordinated groups to develop improved understanding of spillover processes and reproducible materials processing. This includes determining the contributions of bridges and receptor to kinetic limitations, thermodynamically acceptable configurations and the roll catalyst/receptor integration play. Also, scale materials processing to the multi(tens)-gram scale for validation and system testing. Perform very high pressure measurements (> 100 bar) to determine saturation capacities.
  - **Integrate Theory and Experiment:** Iterative, close interactions in the CoE have already taught theoreticians what is possible experimentally, and *vice versa*. Continued work at this interface will increase the rate of discovery and synthesis of viable materials.
- **Materials Down Select:** After down selecting, allocate resources focused on completing work on selected materials to demonstrate their potential to meet DOE 2010 and 2015 system targets and to provide performance properties for system design. Also identify potential cost effective and scalable processing that will produce the hydrogen storage materials with access to the high density of enhanced binding energy sites.
- **Provide Recommendations:** Provide DOE with a comprehensive review of all significant work done, results, lessons learned, and recommendations for future sorption materials development in a report and publication. Key aspects of this review will include material and/or process recommendations for future consideration in engineering system analysis, design, and demonstration, as well as future research and development efforts.
- **Support HSESoE:** Work with HSESoE to select potential materials and provide their intrinsic hydrogen storage properties needed for system engineering design, analysis, and perhaps demonstration.
  - **Sorbent materials approach DOE 2010 targets:** In general, sorbents meet almost all of the DOE hydrogen storage targets. As discussed above, sorbents may greatly improve volumetric capacities, and the HSCoE has developed several materials that may meet DOE's 2010 onboard refueling targets.

More Details in Back-up slides and in partner presentations.

Back-up Slides

Approach to Performing R&D

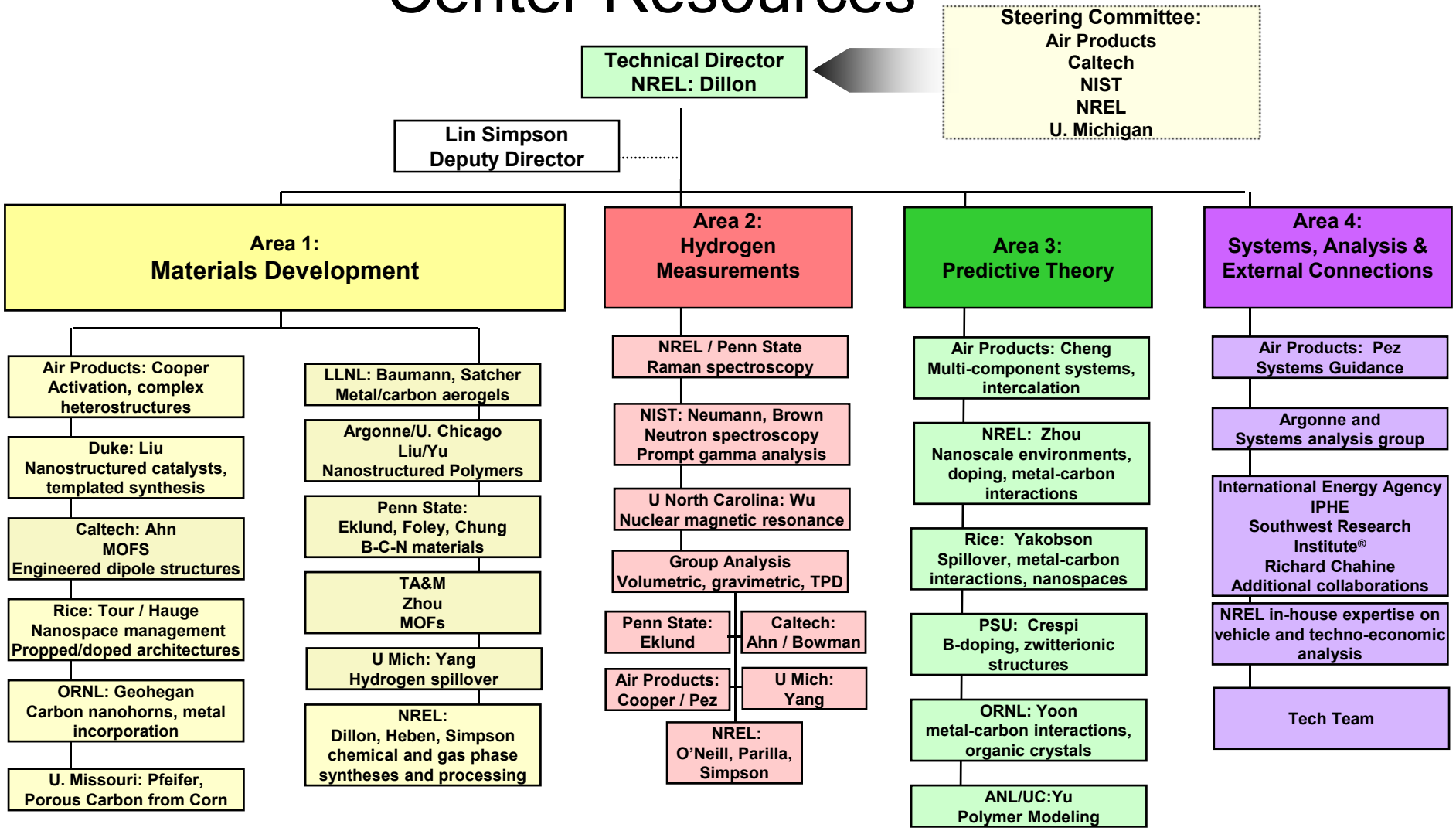
DOE Hydrogen Sorption CoE



9 universities, 5 government labs, 1 industrial partner

Approach to Performing R&D

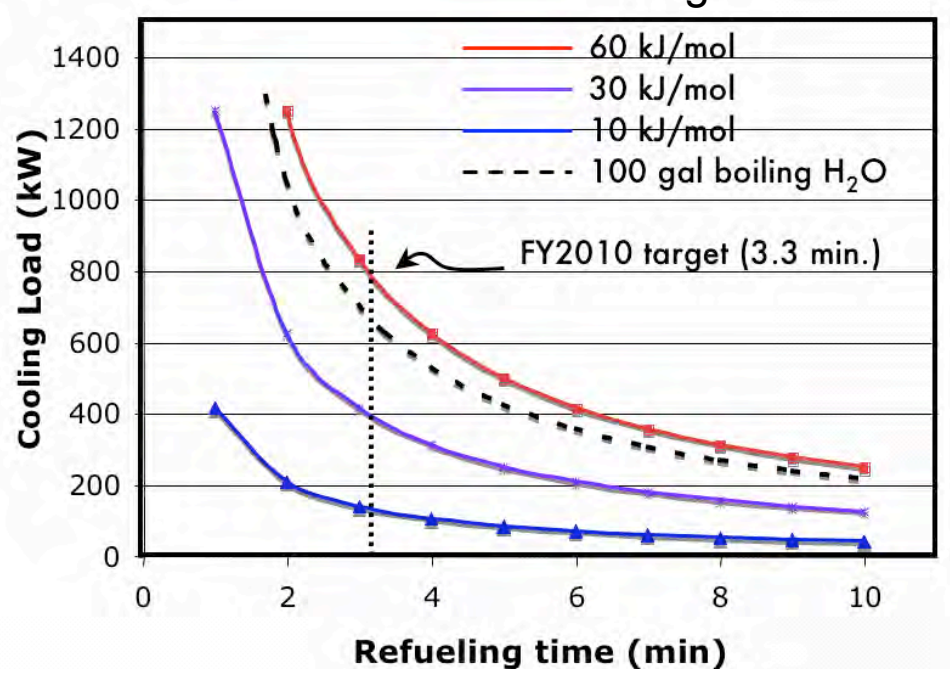
Center Resources



- Level of effort in Materials >> Measurements > Theory (~4:~1.5 :~1)
- No significant effort in producing 1 kg system in agreement with new DOE goals

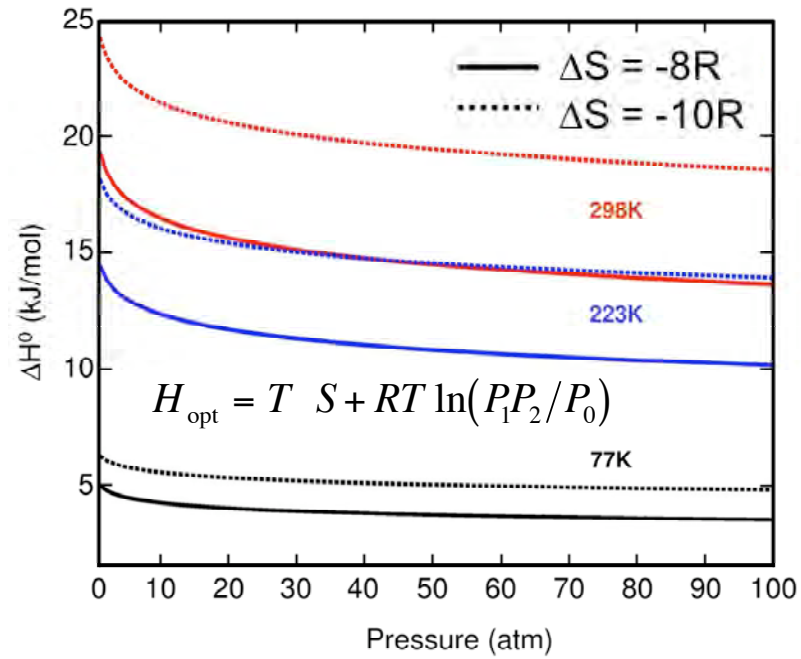
Importance of the Enthalpy for RT Operation

Heat removal challenge



Cooling load for 5 kg of adsorbed H_2 for different binding

Optimal enthalpy to maximize delivered H_2



After Bhatia & Myers, *Langmuir* **2006,** 22, 1688.

- Heat removal with loading 5 kg of H_2 adversely impacts system capacities (heat exchangers) and refueling rates.
- The enthalpy should be the minimized for heat removal but increased for capacity at high tempertures and lower pressures.
- Sorbent materials offer the highest round trip (charge/discharge) energy efficiencies.
- High efficiencies are necessary for any technology to be viable.

Charge to P_2 and discharge to P_1 (1.5 atm)
Entropy values for theoretical slit pore (-8R) and intercalated graphite (-10R).

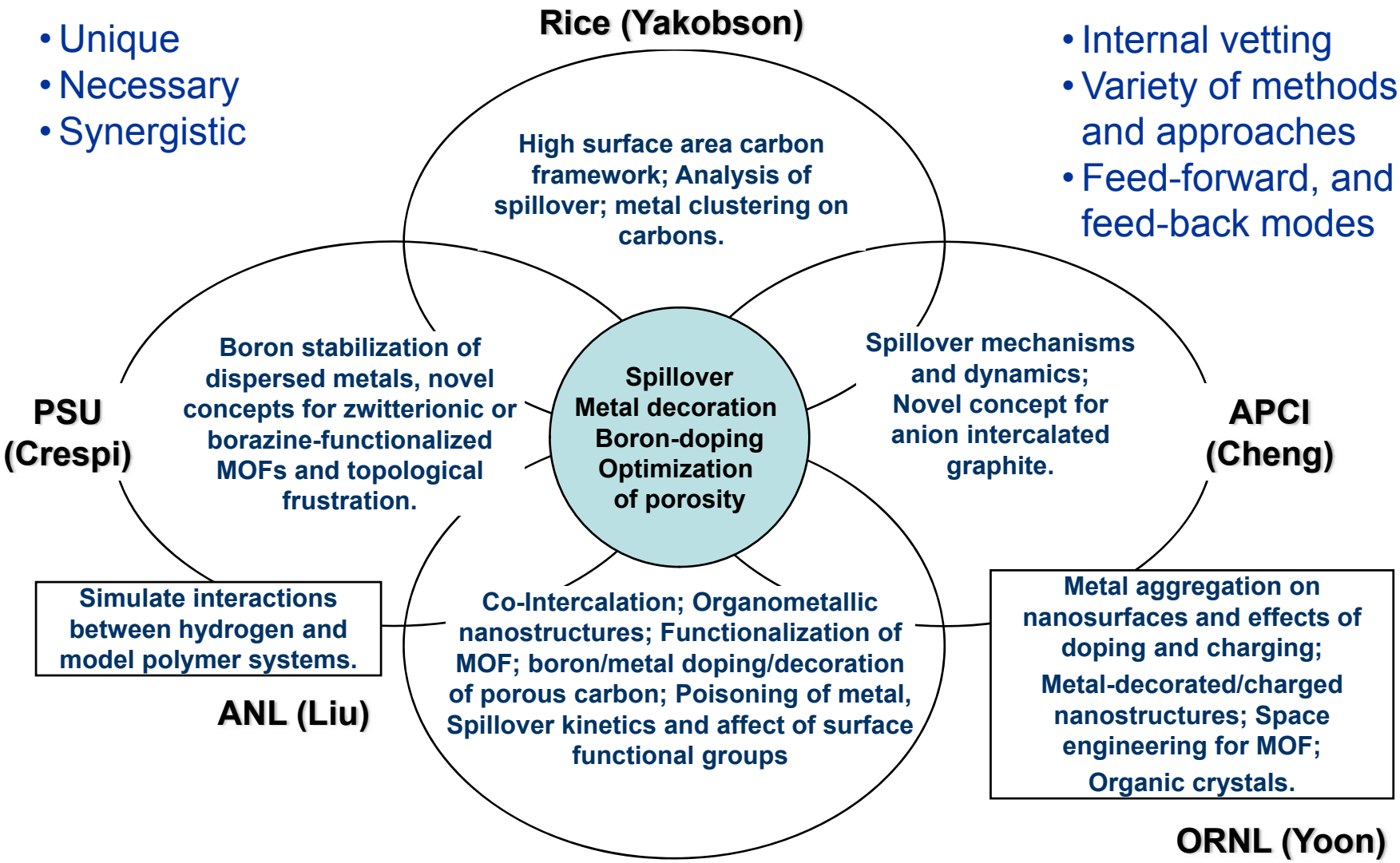
- The binding energy of physisorbed hydrogen is ~ 4-6 kJ/mol H_2 requiring tank operation at 77 K.
- Adsorption at 298 K requires a minimum binding energy of ~ 15 - 20 kJ/mol H_2.

Onboard refueling dictates that the enthalpy of H_2 adsorption be minimized. Sorbent materials offer the most viable path for onboard refueling, with enthalpies between 5 and 20 KJ/mol.

Theory is Coordinated Across the RCs

- Unique
- Necessary
- Synergistic

- Internal vetting
- Variety of methods and approaches
- Feed-forward, and feed-back modes



NREL/CoE Theory Coordinator: Zhao

Down Select Criteria for Each RC

Down-Select Criteria for Engineered Nanospace:

1. The material's gravimetric storage capacity should be approximately 0.03 kgH_2/kg with a volumetric storage capacity of approximately 0.03 kg H_2/L with a possible temperature range of 77 - 200 K and a pressure range of 30 - 100 bar, with a *clear potential* for further improvement.
2. The high-pressure adsorption isotherm should be >80% reversible, i.e., at least 80% of the stored hydrogen is desorbed or discharged between 77 - 200 K, at nominal fuel cell operating pressures.
3. The desorption or discharge rate at 77 - 200 K should meet or be within 90% of the DOE discharge rate target of 0.02 g/s/kW.
4. The charge rate at 77 - 200 K should meet or be within 90% of the DOE target of 3 minutes for 5 kg H_2.
5. Material cost projections should be <0.5 system cost targets

Down-select Criteria for Substitution:

1. The initial binding energy should be in the range of 10-25 kJ/mol, and the material should operate within a temperature range of 77 - 353 K and pressure range of 30 - 100 bar. There should be a *clear potential* for gravimetric and volumetric capacity optimization.
2. The high-pressure adsorption isotherm should be >80% reversible, i.e., at least 80% of the stored hydrogen is desorbed or discharged between 77 - 353 K, for nominal fuel cell operating pressures.
3. The desorption or discharge rate at 77 - 353 K should meet or be within 90% of the DOE discharge rate target of 0.02 g/s/kW.
4. The charge rate at 77 - 353 K should meet or be within 90% of the DOE target of 3 minutes for 5 kg H_2.
5. Material cost projections should be <0.5 system cost targets

Down-select Criteria for Strong Binding:

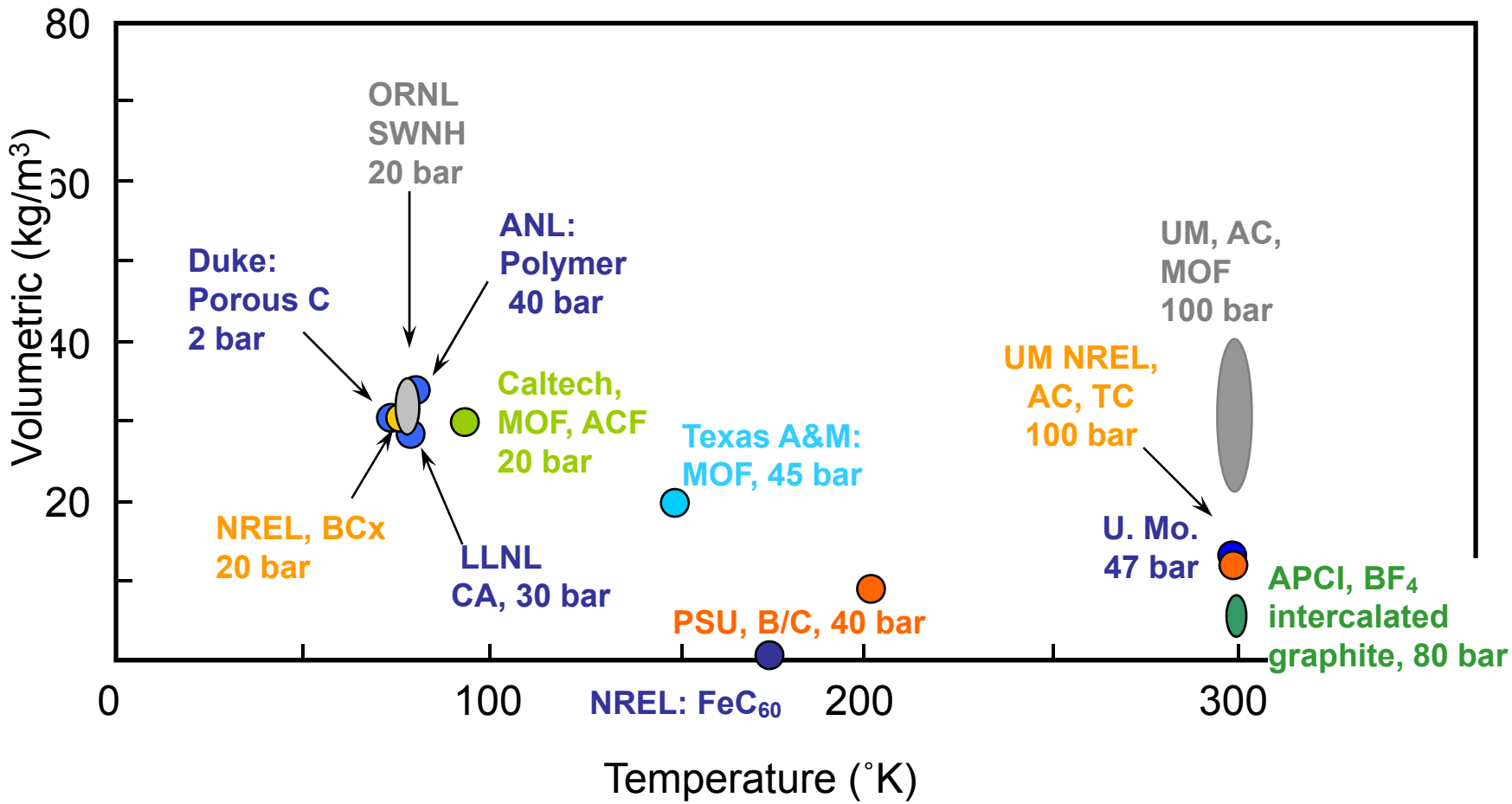
1. The initial binding energy should be in the range of 10-25 kJ/mol, and the material should operate within a temperature range of 77 - 353 K and pressure range of 30 - 100 bar. There should be a *clear potential* for gravimetric and volumetric capacity optimization.
2. The high-pressure adsorption isotherm should be >80% reversible, i.e., at least 80% of the stored hydrogen is desorbed or discharged between 77 - 353 K, for nominal fuel cell operating pressures.
3. The desorption or discharge rate at 77 - 353 K should meet or be within 90% of the DOE discharge rate target of 0.02 g/s/kW.
4. The charge rate at 77 - 353 K should meet or be within 90% of the DOE target of 3 minutes for 5 kg H_2.
5. Materials cost projections should be <0.75 system cost targets

Down-select Criteria for Spillover:

1. The material's gravimetric storage capacity should be approximately 0.01 kgH_2/kg with a volumetric storage capacity of approximately 0.01 kg H_2/L with a possible temperature range between 298 - 353 K at 100 bar, with a *clear potential* for further improvement.
2. The high-pressure adsorption isotherm should be >80% reversible, i.e., at least 80% of the stored hydrogen is desorbed or discharged with a temperature that does not exceed 353 K, for a nominal fuel cell operating pressure.
3. The desorption or discharge rate at 298 - 353 K should meet or be within 80% of the DOE discharge rate target of 0.02 g/s/kW.
4. The charge rate at 298 - 353 K should not exceed 10 hours for a full charge of 5 kg H_2.
5. Materials cost projections should be <0.75 system cost targets

Sites with Enhanced Binding Energy

Volumetric Capacity Versus Charge/Discharge Temperature



Difficult to engineer materials with high density of enhanced binding energy sites. Need to work with HSECoE to determine viable temperature range.