U.S. DEPARTMENT OF ENERGY

2006 Annual DOE Hydrogen Program Merit Review

Hydrogen Storage

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[1] Retired, on assignment to DOE, Washington DC

Outline

- Challenges
  - Goals and Targets
- Strategy
  - Focus on Materials-based Technologies
- Results: Progress in the last year
  - R&D Examples
  - Programmatic Accomplishments
- Future Plans

Hydrogen Storage: The "Grand Challenge"

On-board hydrogen storage to meet all performance (wt, vol, kinetics, etc.) , safety and cost requirements and enable a more than 300 mile driving range.

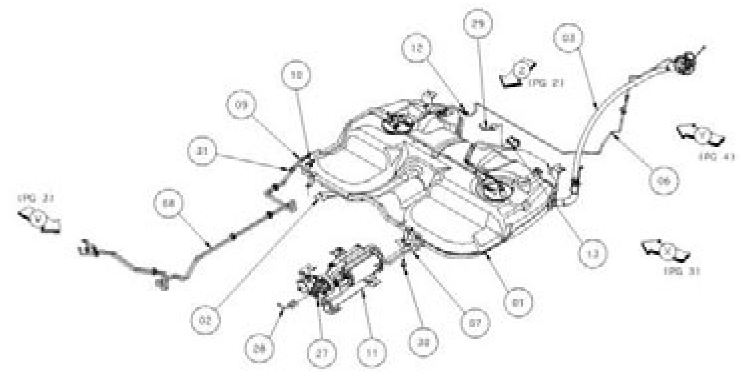
Targets	2010	2015
System Gravimetric Capacity (net)= "specific energy"	**6 wt.%** (7.2 MJ/kg) (2.0 kWh/kg)	**9 wt.%** (10.8 MJ/kg) (3.0 kWh/kg)
System Volumetric Capacity (net)= "energy density"	**1.5 kWh/L** (5.4 MJ/L) (45 g/L)	**2.7 kWh/L** (9.7 MJ/L) (81 g/L)
Storage system cost	**$4/kWh** (~$133/kg H_2)	**$2/kWh** ($67/kg H_2)

More targets and explanations at www.eere.energy.gov/hydrogenandfuelcells/

Targets are for Storage System

Reminder:
<u>System</u>
Targets

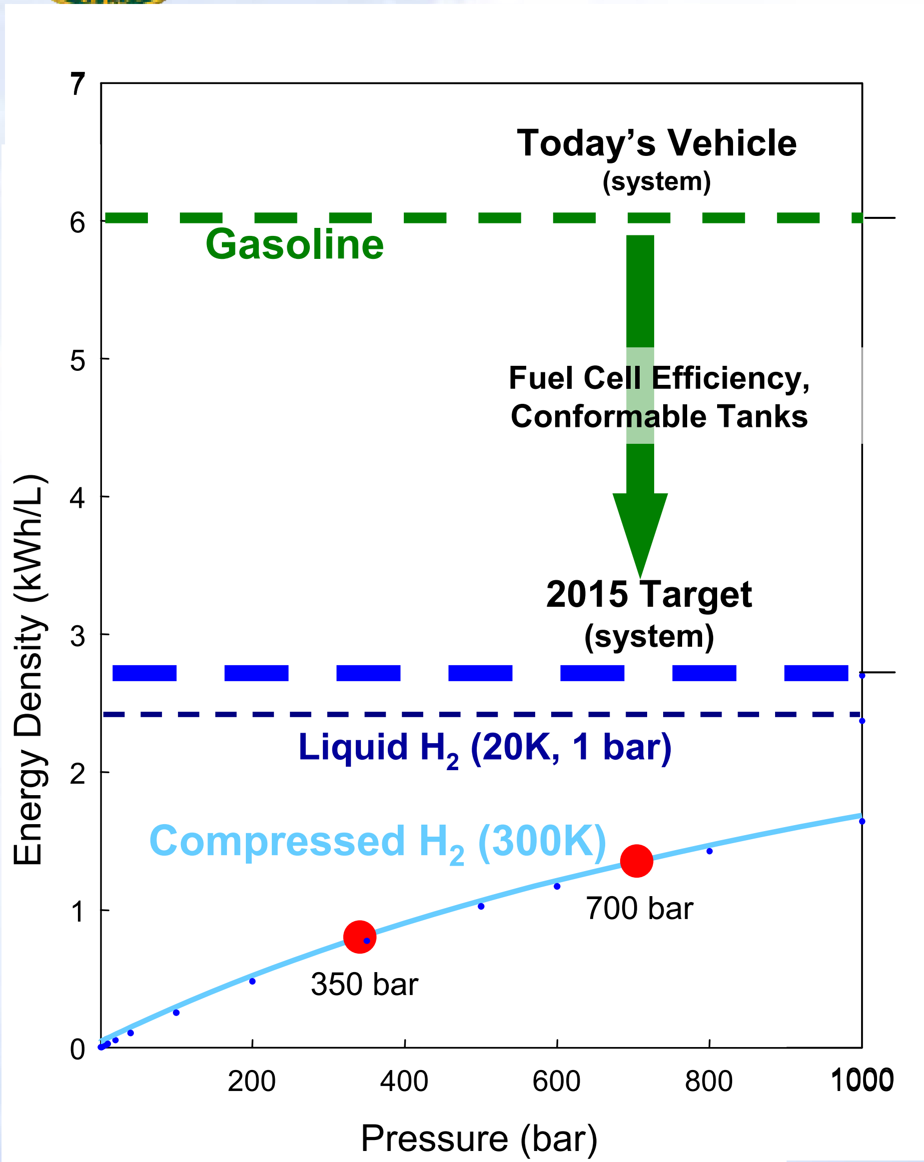
Today's gasoline tank system:

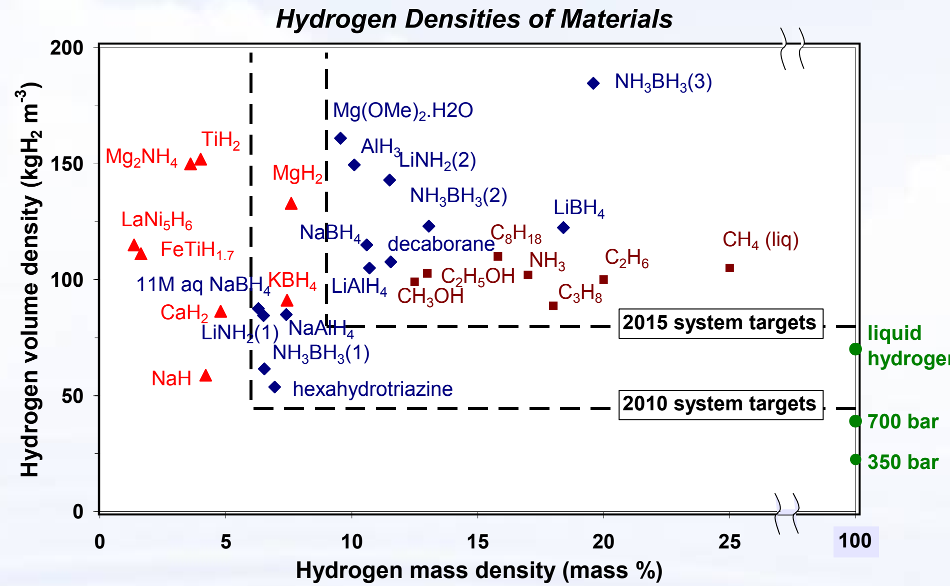


System includes material, tank, and balance of plant- e.g. insulation, sensors, regulators, first charge, any byproducts/reactants, etc.

Material capacities must be higher!

Energy Density (Volumetric Capacity) is Critical!



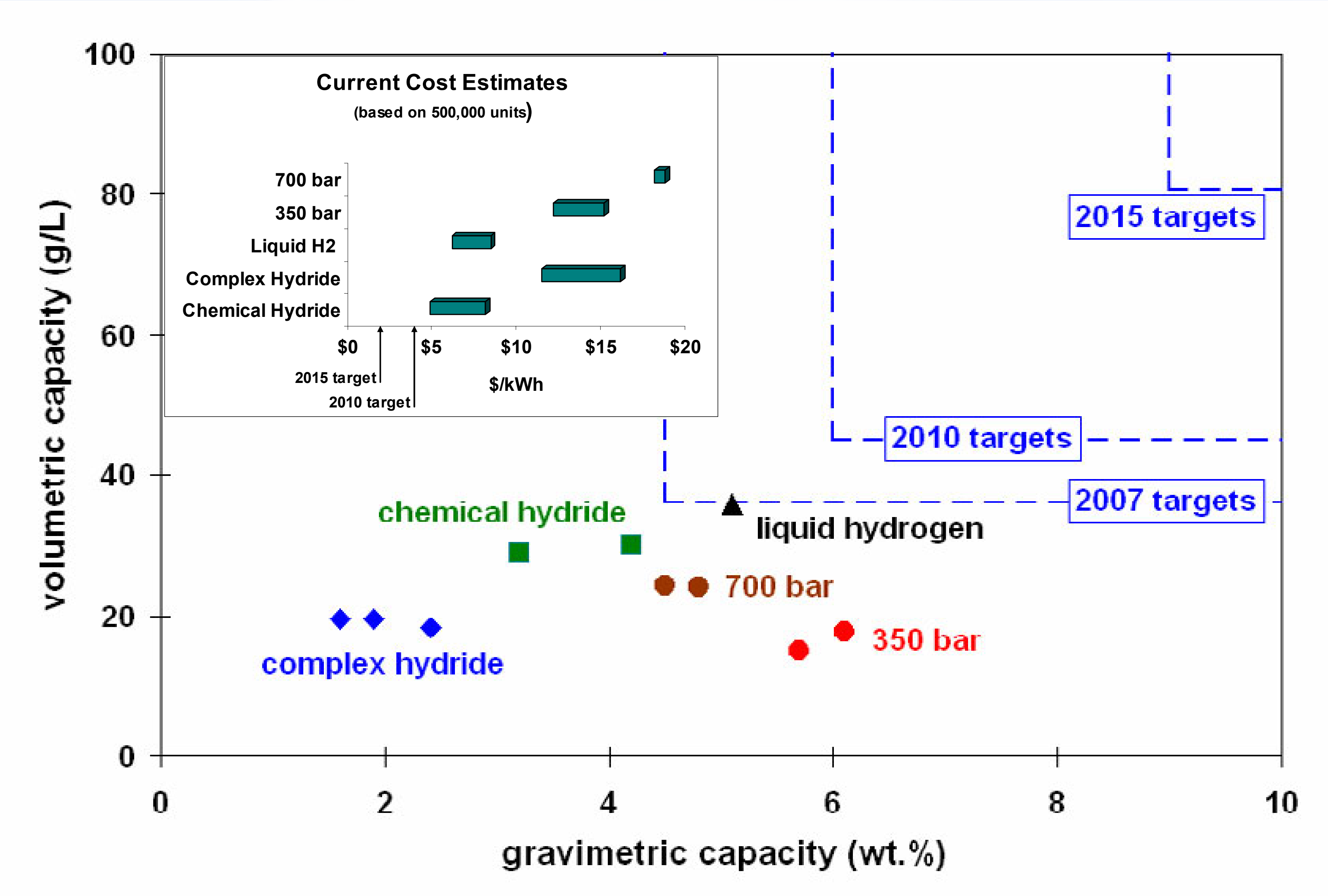


Select materials with capacities higher than system targets

See http://www.eere.energy.gov/hydrogenandfuelcells/storage/current_technology.html

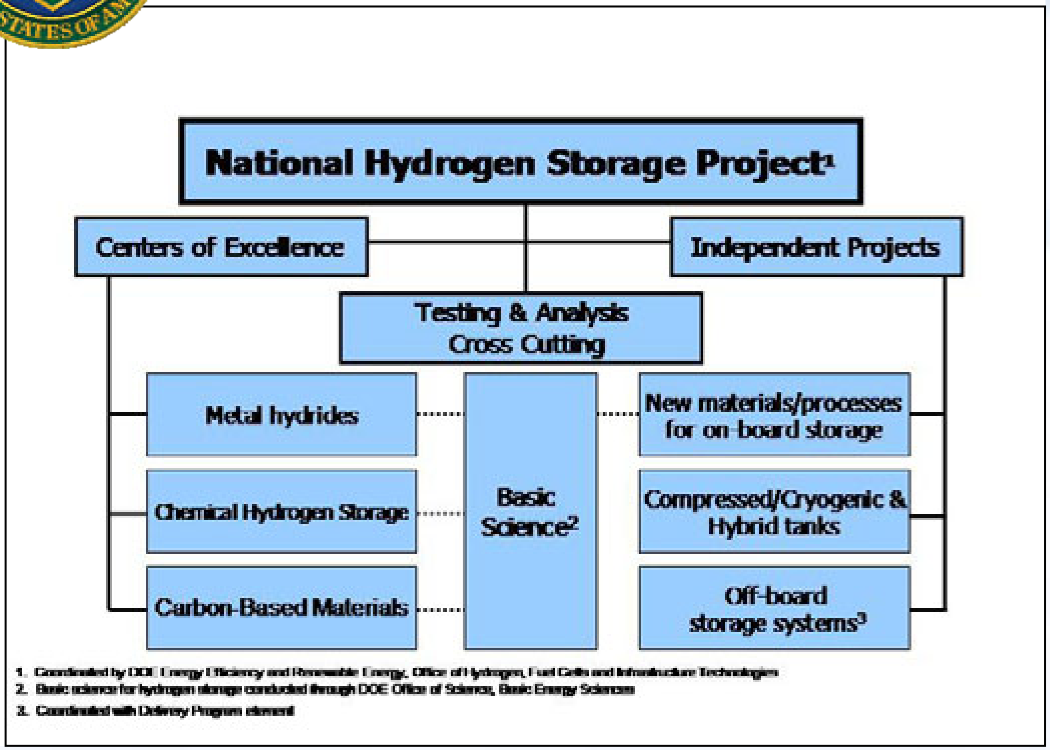
Current Status

No storage technology meets 2010 or 2015 targets

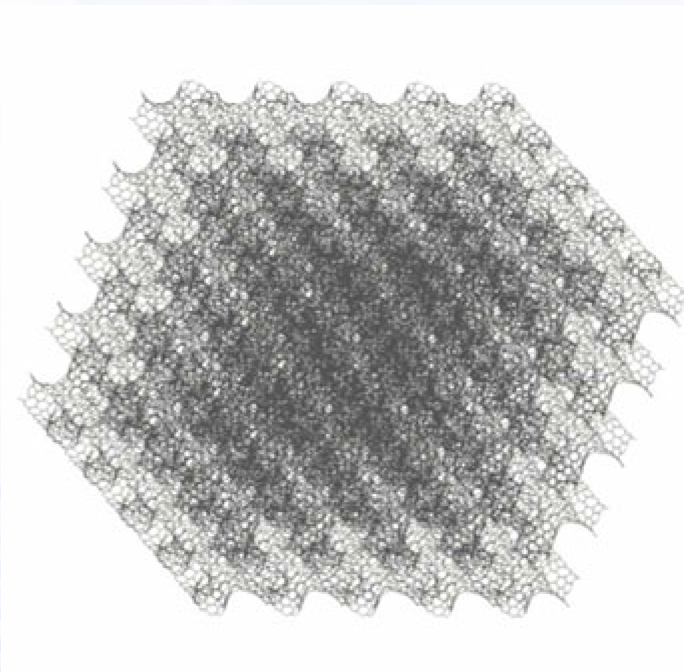


Note: Estimates from developers. To be periodically updated.
Costs exclude regeneration/processing. Complex hydride system data projected. Data points include analysis results.

Strategy and Program Plans



- **Focus is materials-based technologies**
  - **Systematic approach**
  - **Robust theory/simulation and rapid screening**
  - **Tailor properties**
  - **Capacity, T, P, energies**



Yacobsen, Rice U.

- **Centers of Excellence** ($5-6M/yr) plus independent projects, launched at $150 M over 5 years (plan- subject to appropriations)
- **~ 40 universities, 15 companies, 10 federal labs** (including 17 new BES awards)
- **Diverse portfolio addresses NAS recommendations**

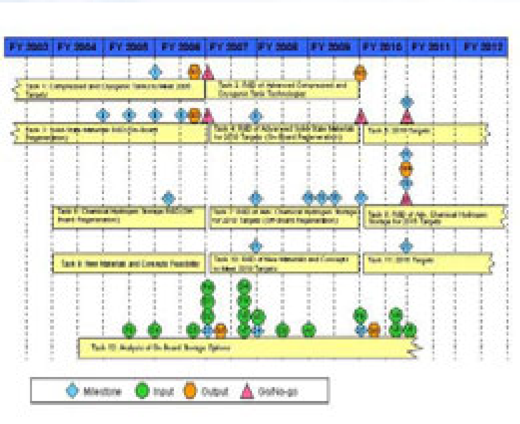
"…DOE should continue to elicit new concepts and ideas, because success in overcoming the major stumbling block of on-board storage is critical for the future of transportation use of fuel cells." (NRC Report,p.44)

Strategy & Results

Broad Portfolio Focused on Materials Technologies

Challenges are technology specific: Pros and Cons for each

Tanks (to 10,000 psi), Chemical hydrides (CH), Metal Hydrides (MH), Carbon/Sorbents (S)



RD&D Plan: Tasks in each area

www.eere.energy.gov/
hydrogenandfuelcells

Thermal Mgmt: Key Issues for MH (CH, C) (applies to Refueling Time and Discharge Kinetics)

Key 2010 Targets:	Tanks	CH	MH	S
Volume (1.5 kWh/L)	H	M	M	M/H
Weight (2.0 kWh/kg)	M	M	M/H	M
Cost ($4/kWh)	M/H	M/H*	M/H	M/H
Refueling Time (3 min, for 5 kg)	L	L	M/H	M
Discharge Kinetics (0.02 g/s/kW)	L	M	M	M
Durability (1000 cycles)	L	M	M	M

H = High (Significant challenge) M/H = Medium/High M = Medium L = Low (minimal challenge)

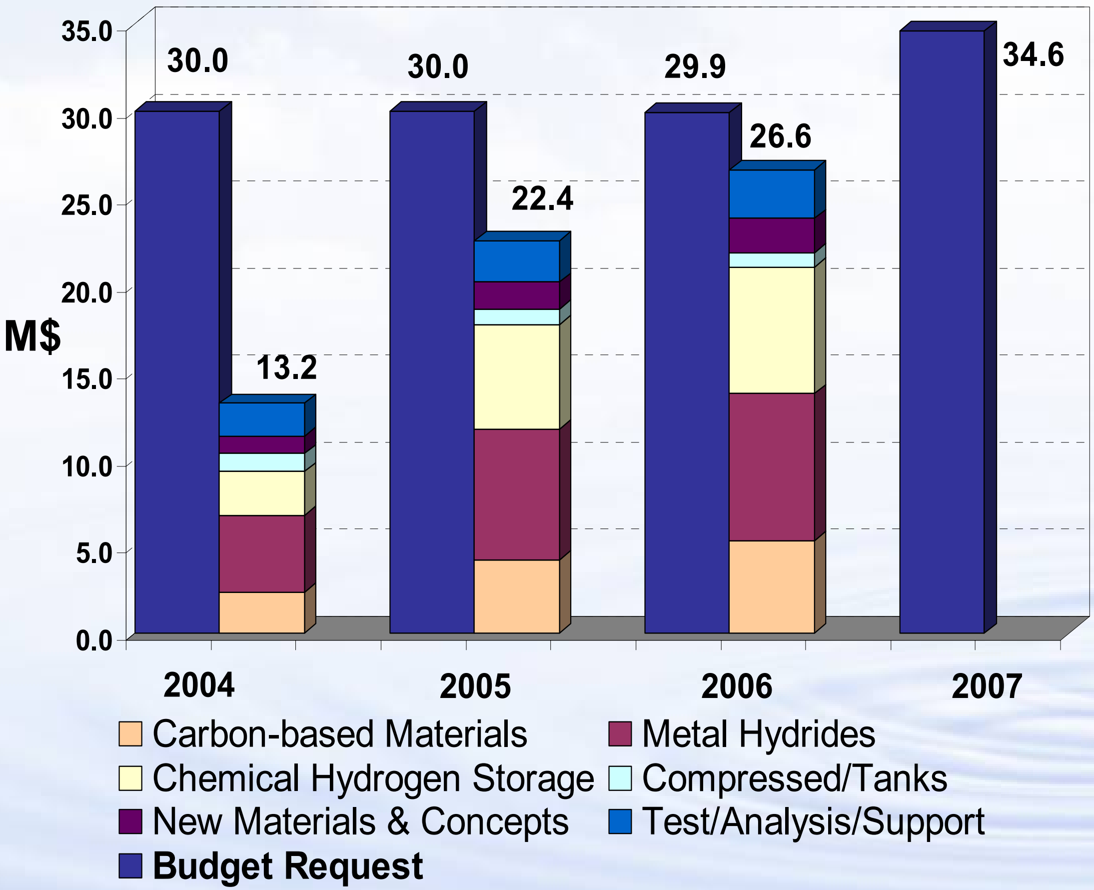
For CH, MH and S- assessment based on potential to meet targets, though systems not yet demonstrated in most cases.

*For CH: Storage system may meet cost but fuel cost of $2-$3/kg is challenge for CH regeneration.

Hydrogen Storage Budget

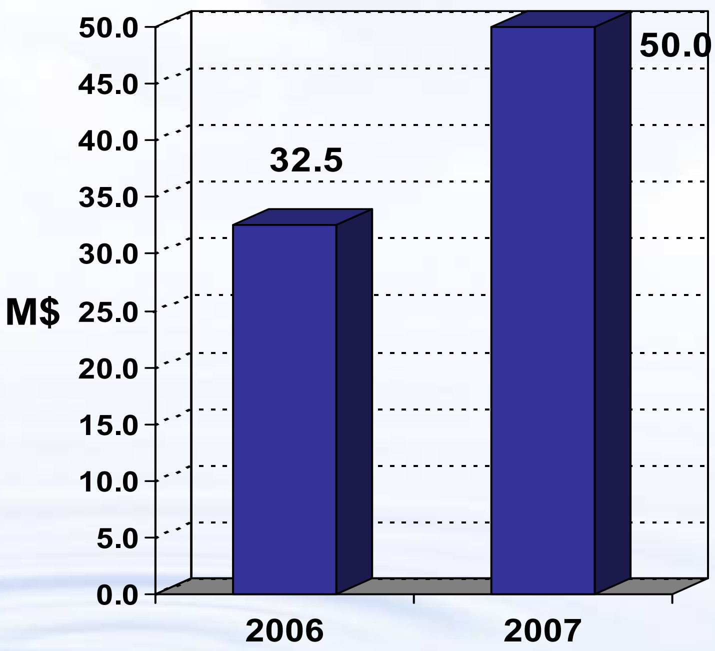
DOE- EERE

FY2007 Budget Request = $34.6M
FY2006 Funding = $26.6M



DOE- Office of Science

FY2007 Budget Request = $50.0M
FY2006 Funding = $32.5M



Planned funding for Basic Science in Hydrogen Storage in FY06: $7.13M

Results: Examples of Progress (2005-2006)

New materials with higher capacities being found

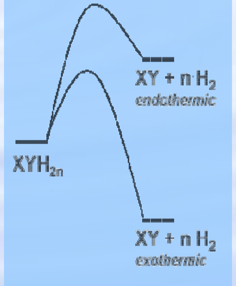
Material Capacities for Hydrogen Storage

Advanced Metal Hydrides	Chemical H_2 Storage	Carbon/ Sorbents & New Materials
Li Mg Amides ~5.5wt%, ~2.8 kWh/L (>200 C) Alane ~7-10 wt%, ~5 kWh/L (<150 C) Li borohydrides >9 wt%, ~3.5 kWh/l (~350 C) Destabilized Binary hydrides ~5-7wt%, ~2-3 kWh/L (250 C) LiMgAlane, M-B-N-H ~ 7-8.8 wt%, > 1.3 kWh/L (~150-340 C)	Phenanthraline/ organic liquids ~7 wt%,~1.8 kWh/L (>150 C) Ammonia Borane/Scaffolds ~6 wt%,~2-4 kWh/L (<100 C)	Metal/carbon hybrids, MetCars 6 to > 8wt%*, ~1.3* kWh/l (*theory) Bridged catalysts IRMOF-8 ~1.8 wt.%,~0.3 kWh/L (room T) Metal-Organic Frameworks IRMOF-177 ~7 wt%, ~1 kWh/L (77 K)

Note: Material capacities only. No balance of plant. Estimates for volumetric capacities.

We are excited by these results but there are still issues…

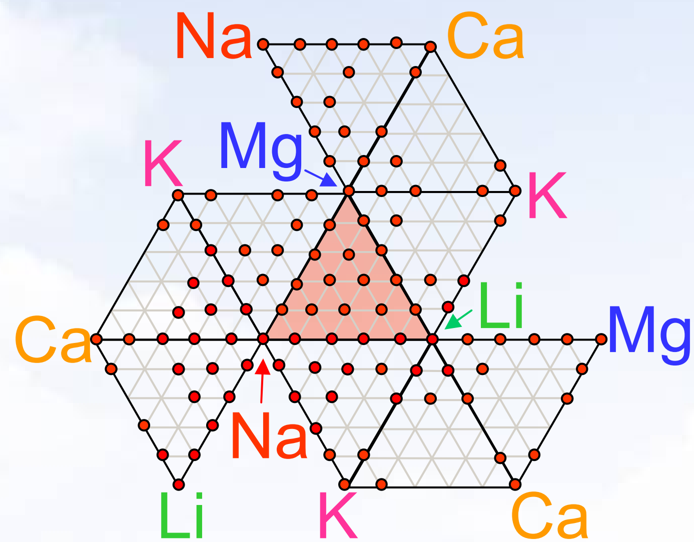
Next steps: Operability (Temperature, pressure, kinetics, etc.)



Results: Advanced Metal Hydrides

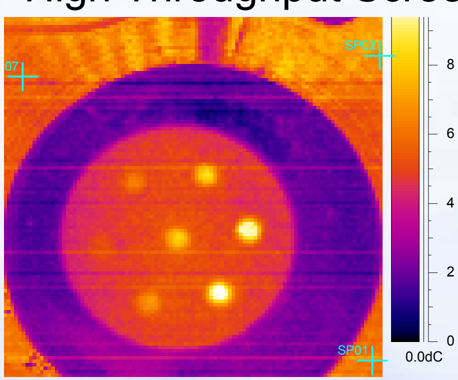
- Rapid Screening: Theory and Experiment
- More than 980 ternary phase systems searched (alkali/alkaline earth alanates)
- No stable mixtures found under UOP conditions (~90 atm)

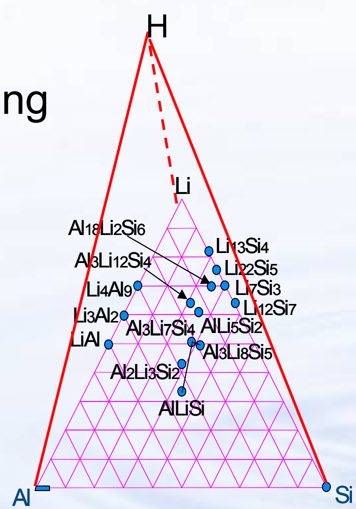
Preliminary Assessment
No alanate mixtures likely to meet DOE targets

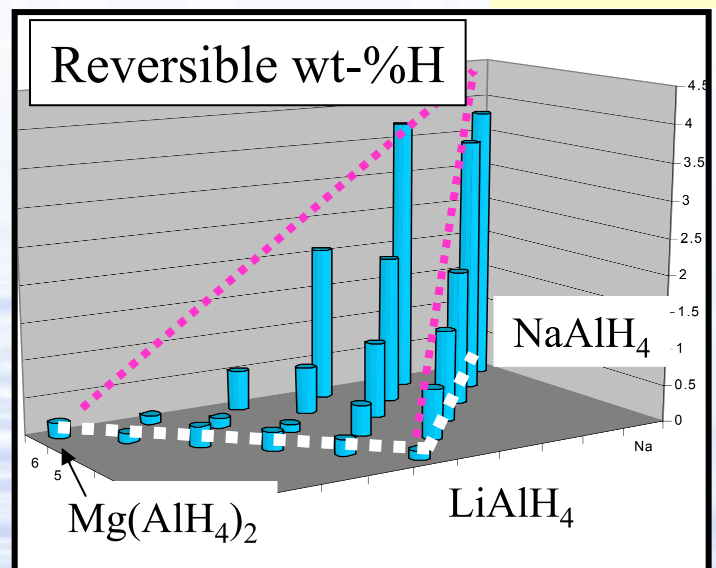


Sachtler, et al, UOP

High Throughput Screening



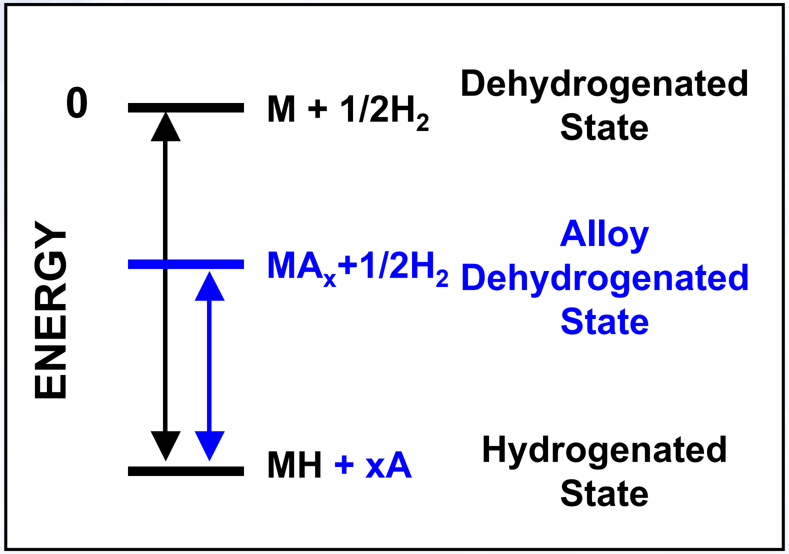


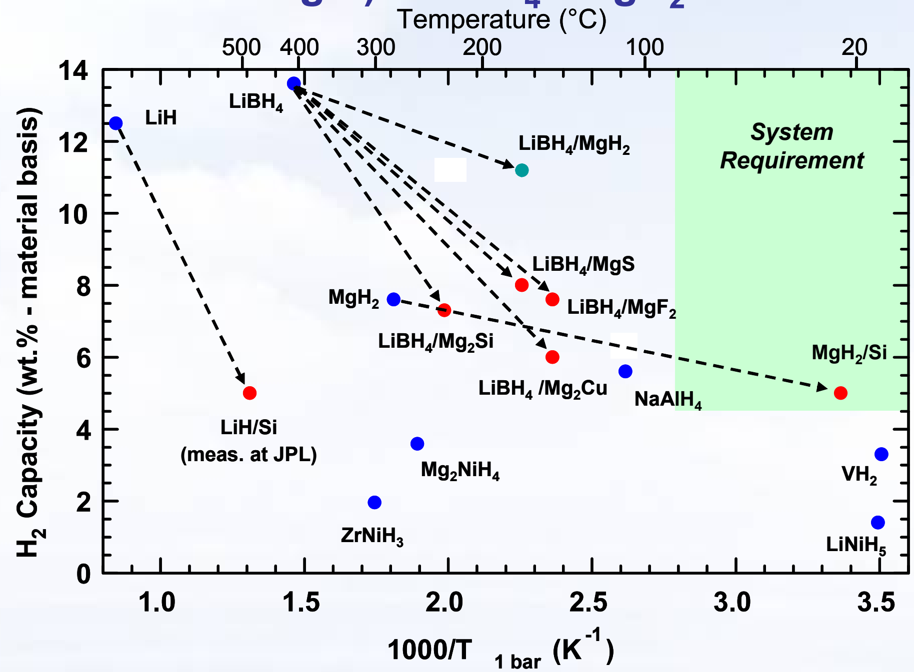


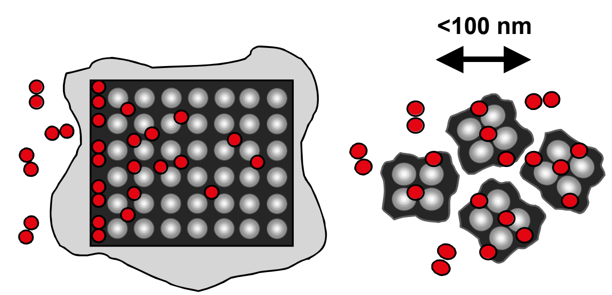
Lemmon, Rubinsztajn, Cui & Zhao (GE)

Results: Destabilized hydrides and nano-engineering

E.g., New system (11.4 wt. % and 0.095 kg/L) – $LiBH_4$ / MgH_2







Long H-diffusion distances in bulk materials: *reduced H-exchange rate*

Short H-diffusion distances in nanoparticles: *fast hydrogen exchange*

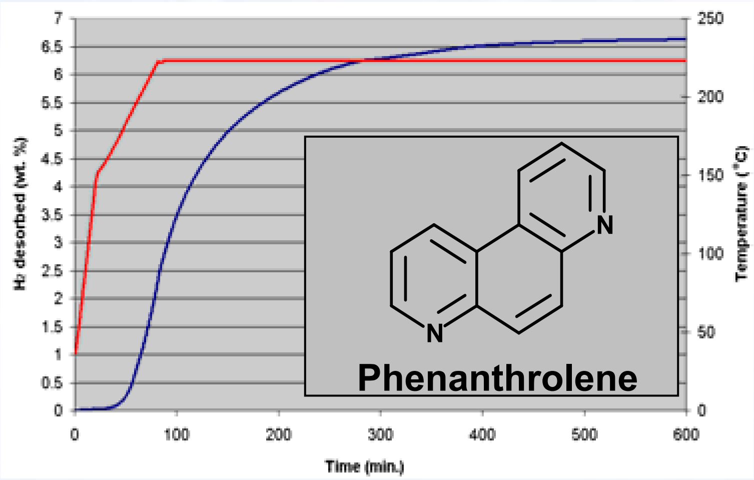
Vajo, Olsen, et al, HRL

- Demonstrated "destabilization" to enable lower T
  - Showed ~9-10 wt.% $LiBH_4/MgH_2$
  - Can reduce T by ~ 240 C
  - But kinetics slow
- Next steps: Enhance kinetics by nano-engineering

J. Vajo, S. Skeith, and F. Mertens, J. Phys. Chem. B, 109, 3719-3722 (2005).

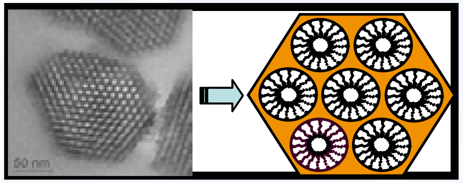
Results: Chemical Hydrogen Storage

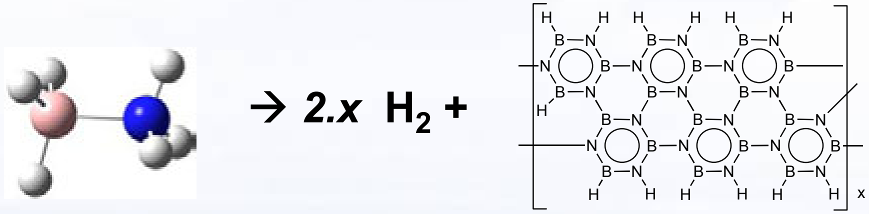
- Organic liquids: >7 wt.%, 69 g/L
  - 1.5 wt% more than FY05
  - > 100 catalysts screened
  - > Dehydrogenation with 10x less Pt in catalysts



Cooper, Pez, et al, Air Products

- NH_3BH_3 in mesoporous scaffolds:
  - >6 wt% material capacity
  - H_2 release at < 80 C
  - Reduced borazine formation



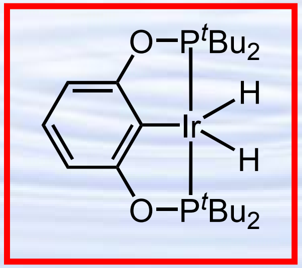


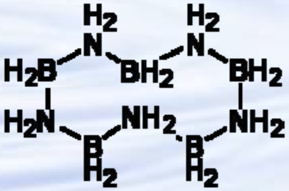
Autrey, Gutowski, et al, PNNL
Chemical CoE

Rapid dehydrogenation catalysts demonstrated

U. of Washington, Chemical CoE

$$H_3NBH_3 \xrightarrow[\text{THF, rt}]{\text{Ir cat.}} 1/5\ [H_2NBH_2]_5 + H_2$$



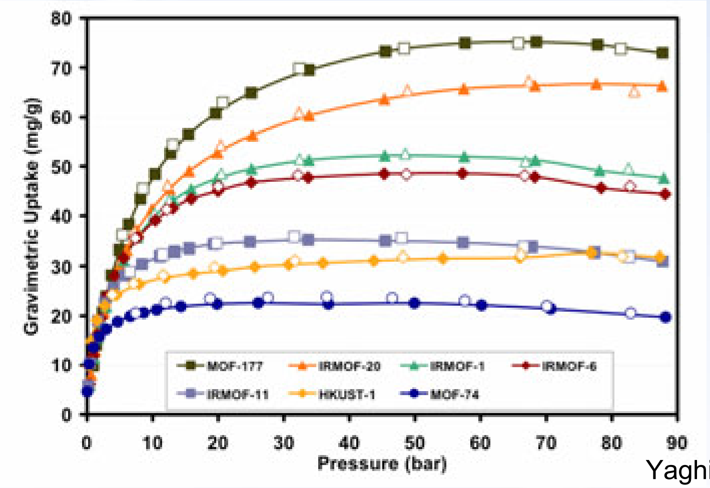


Original catalyst development- Jensen, et al (U HI)

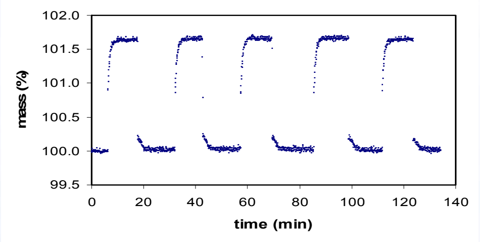
Results: Carbon and Sorbents

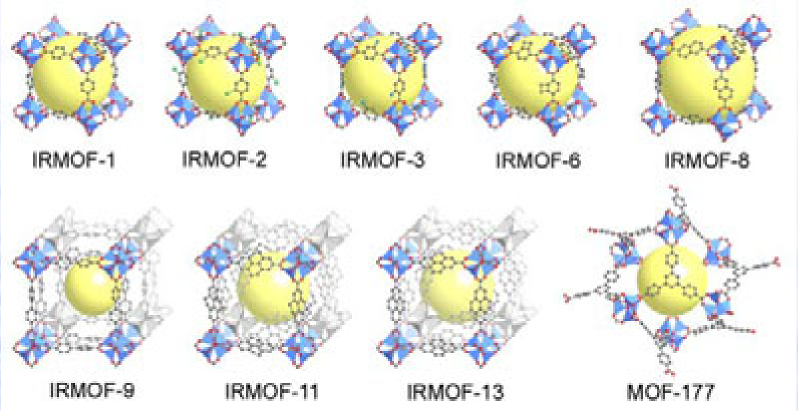
Carbon Center & New Materials:

- >7 wt.% at 77K shown on MOFs (> 30 g/L)
- Several cycles reversibility shown
- Four-fold enhancement in H_2 storage via "spillover"



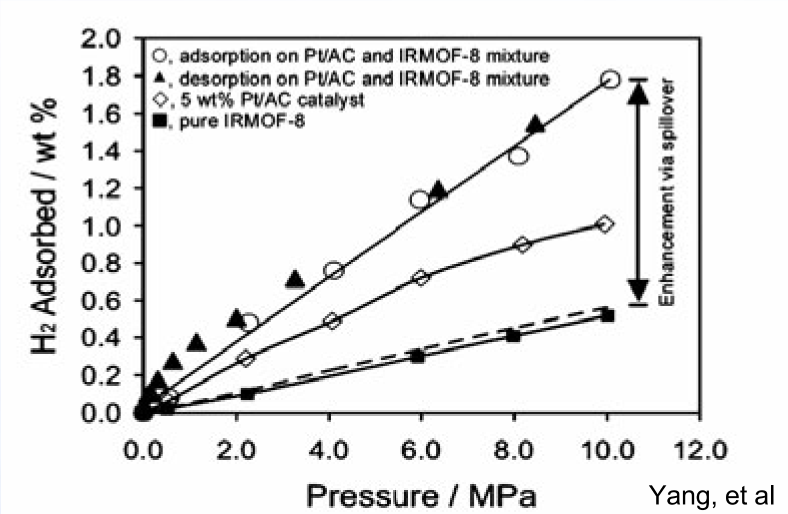
Yaghi, Matzger (UCLA, U MI)





Yaghi, et al

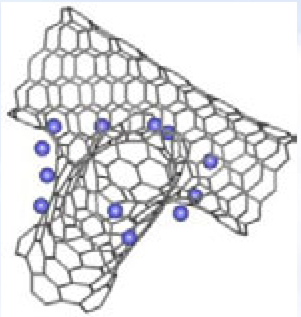
A.G. Wong-Foy, A.J. Matzger, O.M. Yaghi, *JACS* (2006)

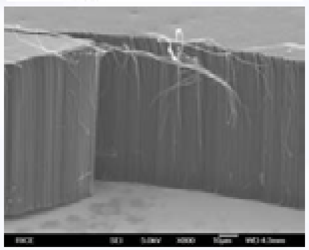


Yang, et al (U MI)

Y. Li and R.T. Yang, *JACS (2006)*

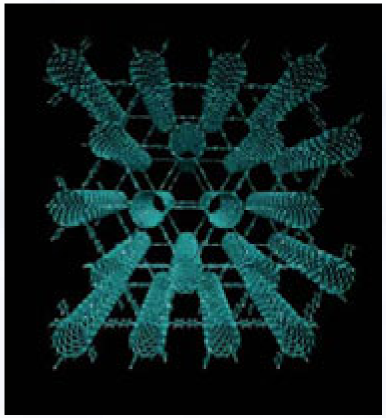
Results: Designing tailored nanostructures





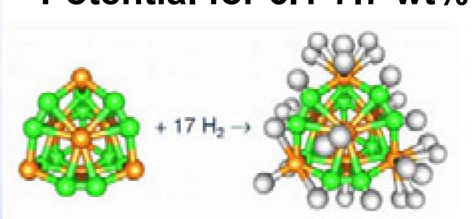
CNT "Carpet"
Tour, et al, Rice U.

Yakobson, Ding, Lin
Rice University
Carbon Center

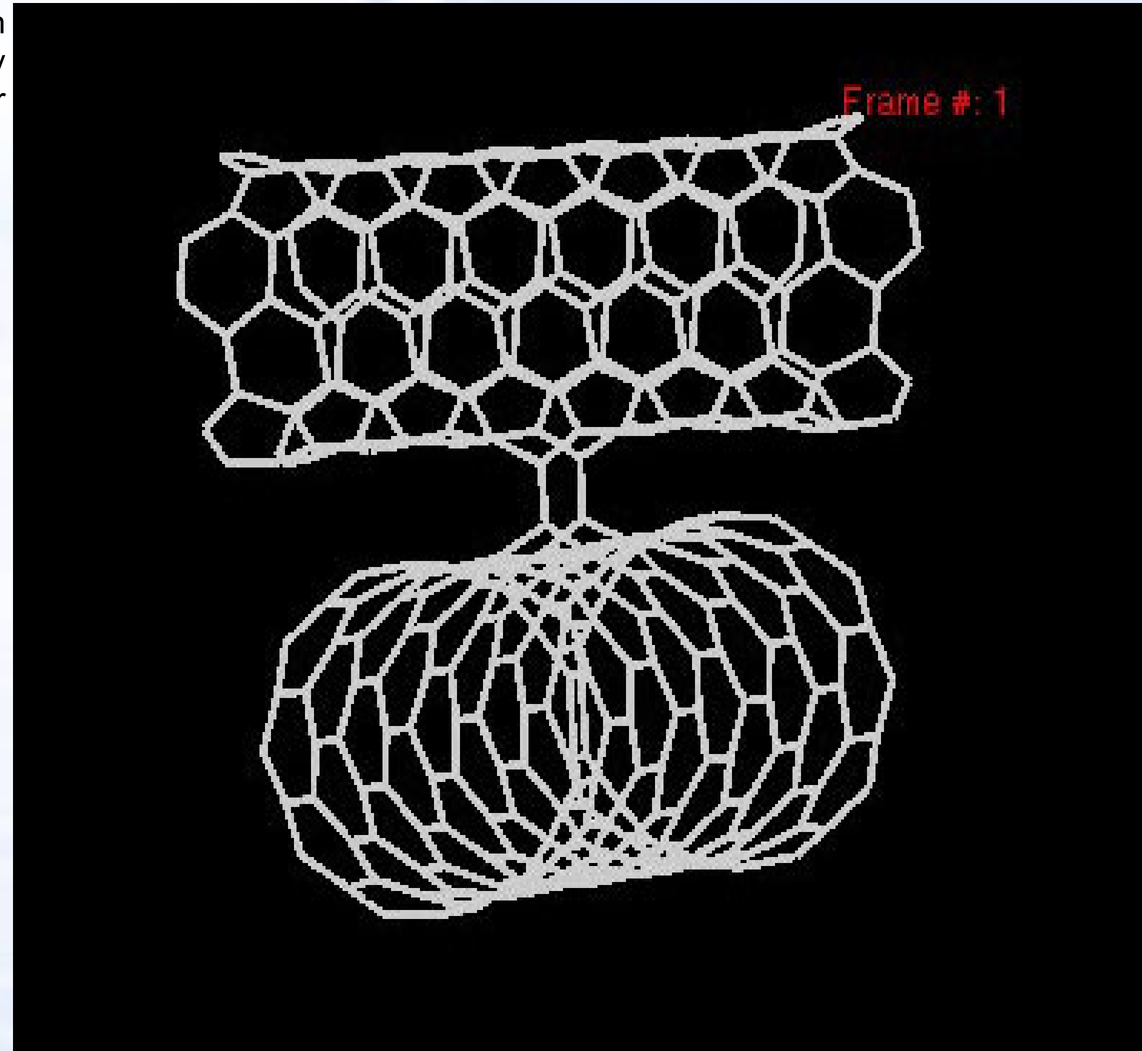


NREL-Carbon Center

Potential for 6.1-7.7 wt%



MetCars
Y. Zhao, A.C. Dillon, Y.-H. Kim, M.J. Heben, S.B. Zhang, in prep



Yakobson, et al

Theoretical modeling conducted to predict optimum structures and storage capacities

Results: Testing and Analysis

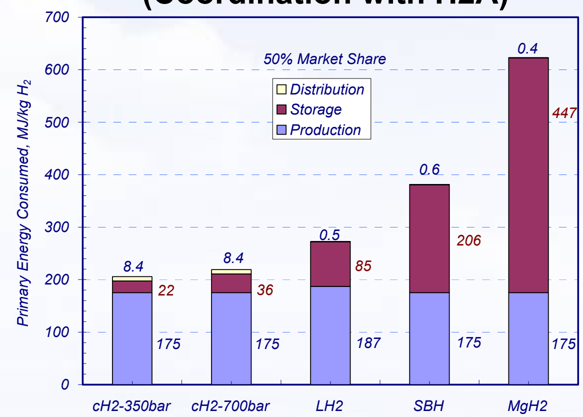
Analysis & modeling underway to determine material property requirements to meet system targets. Preliminary results shown.

Test facility completed, SwRI

R. Page, M. Miller, SwRI

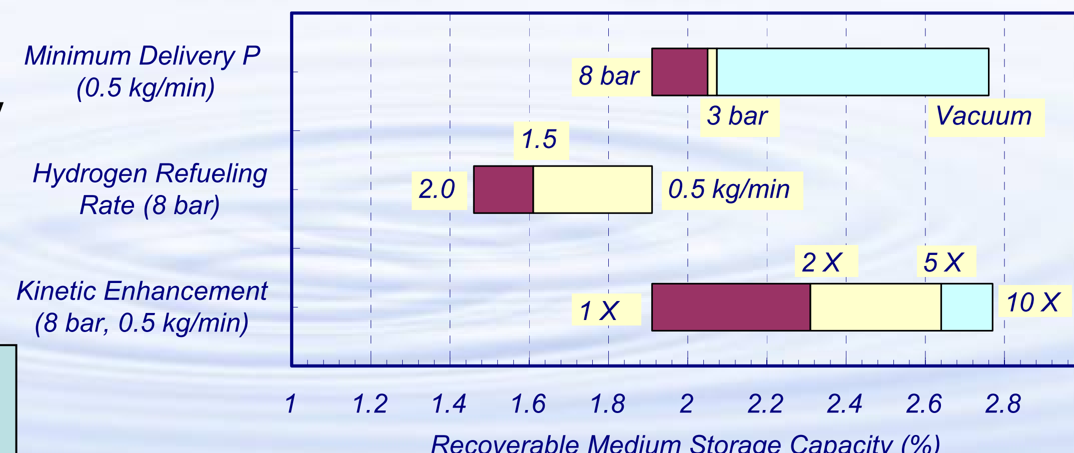
Overall efficiency analyses underway

(Coordination with H2A)



Preliminary estimates based on developer regeneration efficiency analyses

Sensitivity analysis to determine impact of key parameters



R. Ahluwalia, et al, Argonne

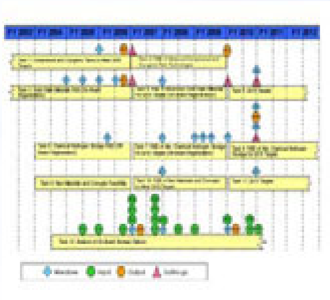
Materials with > 7 wt% likely even for 2007 targets (4.5 wt%)

S. Lasher, et al, TIAX

Storage Systems Analysis Working Group

Programmatic Accomplishments

- IPHE Hydrogen Storage Conference
  - Leveraging global activities
  - See www.iphe.net
- Expanded Basic Science
- Theory Focus Session
  - May 18, 2006
- Updated Targets & Multiyear Plan
  - New versions on web
- Addressing NAS recommendations (e.g. revolving solicitation for new concepts)



FreedomCAR & Fuel Partnership

- Water Availability Model
  - For hydrolysis
- Paper on Ammonia
  - Draft on web for public comment
- Updated Roadmap & Targets
  - New versions on web
- Joint Tech Team meetings
  - Defining requirements

See: www.eere.energy.gov/hydrogenandfuelcells/

Hydrogen Storage – Future Plans

Centers of Excellence Launched

IPHE Hydrogen Storage Conference Lucca, Italy

Solicitation Released

Ammonia Paper Released for Comment

Pre-Proposals Due

Full Proposals Due

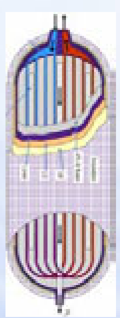
Pre-Proposals Due

2005 | 2006 | 2007

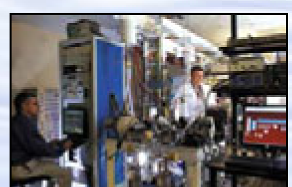
Mar | Jun | Sep | Dec | Mar | Jun | Sep | Dec | Mar

Storage Systems Analysis Working Group Launched

Testing Workshop



Updated Roadmap

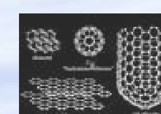


Theory Focus Session

Test Facility Validation

Cryo-compressed Tank Assessment

Go/No Go Single - walled Nanotubes



Release Solicitation *

*Subject to appropriations

Current Solicitations

1) Applied Research and Development (EERE)

– Up to $6M total ($2M planned in FY07, subject to appropriations)

Complements current DOE Centers of Excellence & existing Independent projects:

- – Material discovery
- – Engineering Science (including materials safety properties)
- – Systems, safety and environmental analyses

– 3-6 awards at $200-400k/yr for 2-5 years

– Preproposals due **June 7**

2) Basic Science (Office of Science, BES)

– Up to $52.5M total ($17.5M/yr starting in FY07, subject to appropriations)

- – Novel Materials for Hydrogen Storage
- – Functional Membranes
- – Nanoscale Catalysts

– Preproposals due **July 6**

See http://www.grants.gov or follow links from www.hydrogen.energy.gov

Summary

- New Materials & Concepts are critical- address volumetric capacity, T, P, kinetics, etc. (not just wt. %!)
- Basic science is essential to develop fundamental understanding & complements applied research & development
- Engineering issues need to be considered
  - System issues, thermal mgmt, safety, refueling, testing, etc
- Examples of Essential Capabilities:
  - Modeling & Analysis
  - Combinatorial/high throughput methods
  - Material properties measurements
  - Standardized & accurate testing

For More Information

Hydrogen Storage Team

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New Hire
Carbon/Sorbents, Carbon Center of Excellence
see www.eere.energy.gov/hydrogenandfuelcells/
(closes May 19)

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www.hydrogen.energy.gov

Additional Information

Hydrogen Storage "Grand Challenge" Partners

Centers of Excellence

Metal Hydride Center

National Laboratory:
Sandia-Livermore

Industrial partners:
General Electric
HRL Laboratories
Intematix Corp.

Universities:
CalTech
Stanford
Pitt/Carnegie
Mellon
Hawaii
Illinois
Nevada-Reno
Utah

Federal Lab Partners:
Brookhaven
JPL
NIST
Oak Ridge
Savannah River

Carbon Materials Center

National Laboratory:
NREL

Industrial partners:
Air Products & Chemicals

Universities:
CalTech
Duke
Penn State
Rice
Michigan
North Carolina
Pennsylvania

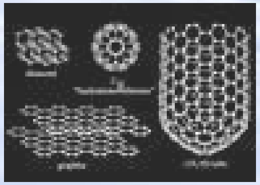
Federal Lab Partners:
Lawrence Livermore
NIST
Oak Ridge

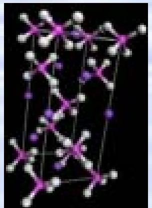
Chemical Hydrogen Center

National Laboratories:
Los Alamos
Pacific Northwest

Industrial partners:
Intematix Corp.
Millennium Cell
Rohm & Haas
US Borax

Universities:
Northern Arizona
Penn State
Alabama
California-Davis
UCLA
Pennsylvania
Washington





Independent Projects

New Materials & Concepts
Alfred University
Carnegie Institute of Washington
Cleveland State University
Michigan Technological University
TOFTEC
UC-Berkeley
UC-Santa Barbara
University of Connecticut
University of Michigan
University of Missouri

High-Capacity Hydrides
UTRC
UOP
Savannah River NL

Carbon-based Materials
State University of New York
Gas Technology Institute
UPenn & Drexel Univ.

Chemical Hydrogen Storage
Air Products & Chemicals
RTI
Millennium Cell
Safe Hydrogen LLC

OffBoard, Tanks, Analysis & Testing
Gas Technology Institute (w/Delivery)
Lawrence Livermore
Quantum
Argonne Nat'l Lab & TIAX LLC
SwRI