2005 Annual DOE Hydrogen Program Merit Review

Hydrogen Storage

Grace Ordaz

John Petrovic[1]

Carole Read

Sunita Satyapal

Basic Science Research Needs presented by George Thomas

ST1

[1] Laboratory Fellow, change of station assignment to DOE HQ

- Overview & Approach
  - Challenges & Targets
  - Basis for Targets & Current Status
  - Research Portfolio & RD&D Plan
- Status & Key Accomplishments
  - Technology Progress
  - Key Activities & Outputs
  - Program Planning/Coordination
- Future Plans
  - Budget
  - Upcoming Solicitation & RD&D Needs

Hydrogen Storage: Challenges & Targets

Challenge: **How to store hydrogen on-board to meet performance (wt, vol, kinetics, etc.) , safety and cost requirements and enable > 300 mile range, without compromising passenger/cargo space.**

Targets: **Developed through** FreedomCAR & Fuel Partnership

These Are System Targets

Material capacities must be higher!

	2010	2015
System Gravimetric Capacity= Specific Energy (net)	2.0 kWh/kg (7.2 MJ/kg) (6 wt%)	3.0 kWh/kg (10.8 MJ/kg) (9 wt%)
System Volumetric Capacity=Energy Density (net)	1.5 kWh/L (5.4 MJ/L) (0.045 kg/L)	2.7 kWh/L (9.7 MJ/L) (0.081 kg/L)
Storage system cost	$4/kWh	$2/kWh

Explanations at www.eere.energy.gov/hydrogenandfuelcells/

Focus is on capacity: but many other requirements…

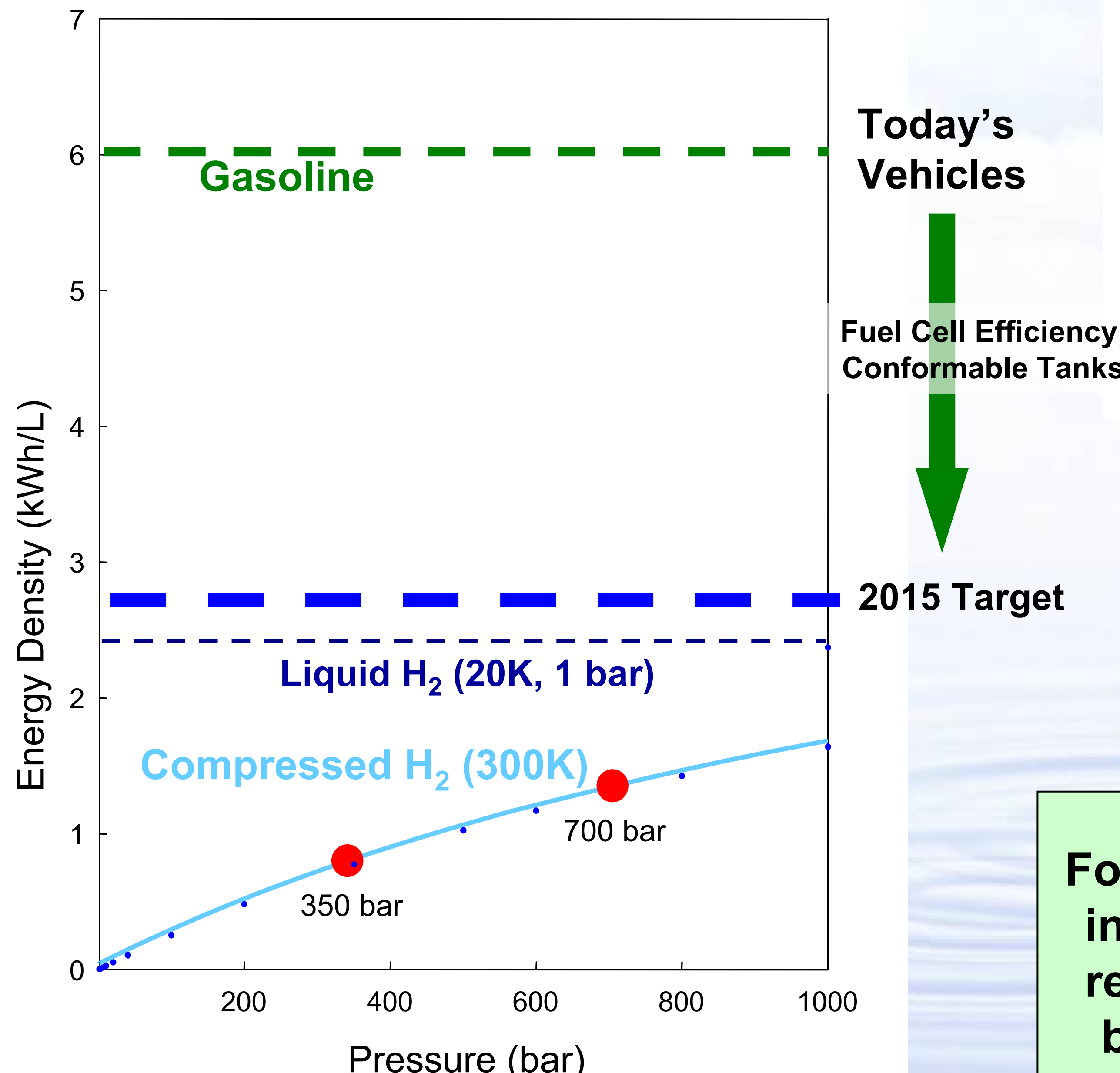
Primary 2005 targets achieved with high P/LH_2 → 2007 → For materials-based systems

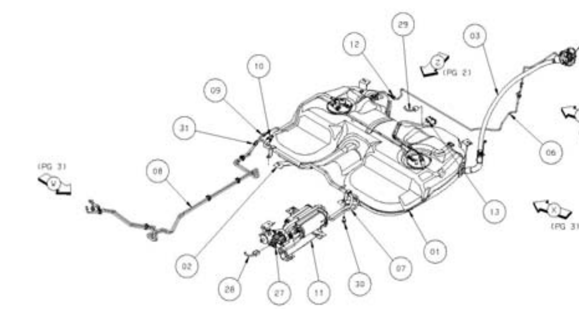
Parameter	Units	2005(7)	2010	2015
Specific energy net	kWh/kg	1.5	2.0	3.0
Energy density net	kWh/L	1.2	1.5	2.7
Storage system cost	$/kWh	6	4	2
Cycle life (25-100%)	cycles	500	1000	1500
Cycle life variation	% of mean (min) @ % confidence	N/A	90/90	99/90
Max delivery temp.	°C	85	85	85
Minimum delivery pressure of H_2 from tank, FC=fuel cell, I=ICE	atm (abs)	8 FC 10 ICE	4 FC 35 ICE	3 FC 35 ICE
Start time to full flow @ 20 °C	sec	4	4	.5
System fill time (for 5 kg)	min	10	3	2.5
Loss of useable hydrogen	(g/h)/kg H_2 stored	1	0.1	0.05
Permeation and leakage	Scc/h	Federal enclosed-area safety standard		
Toxicity		Meets or exceeds applicable standards		
Safety		Meets or exceeds applicable standards		

Current Focus (specific energy net, energy density net, storage system cost)

These are just some, more available at www.eere.energy.gov/hydrogenandfuelcells/

Energy Density is Critical

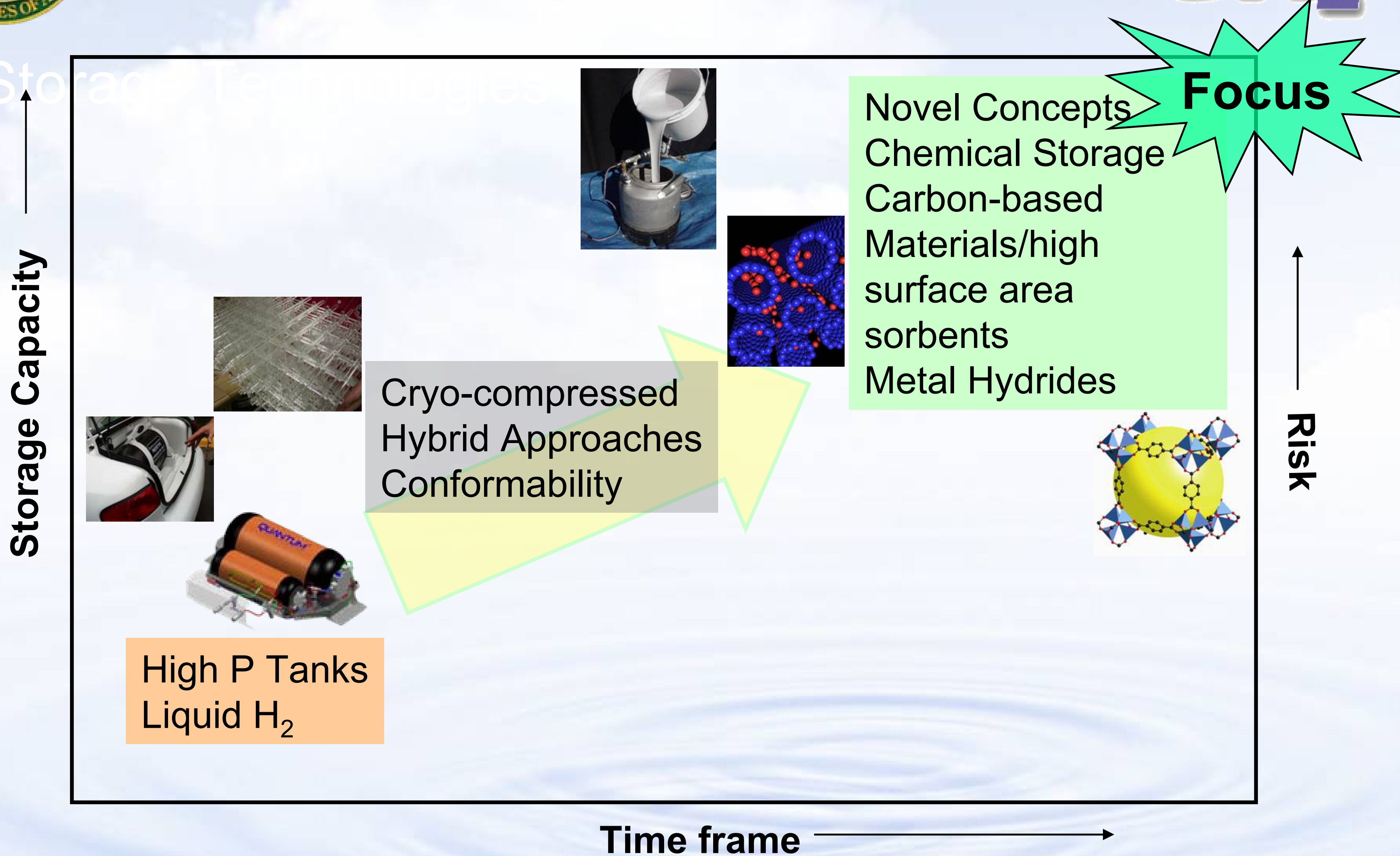




Today's gasoline "tank": fuel tank, fuel filler tubes, gas cap, hoses, fuel lines , fuel pump, fuel filter, carbon vapor canister, leak detection device, purge control solenoid, rollover check valve, tank hanger straps, clips, and other small fasteners

For Hydrogen Systems: Also include insulation, sensors, regulators, first charge, any byproducts/reactants, etc.

Research Areas

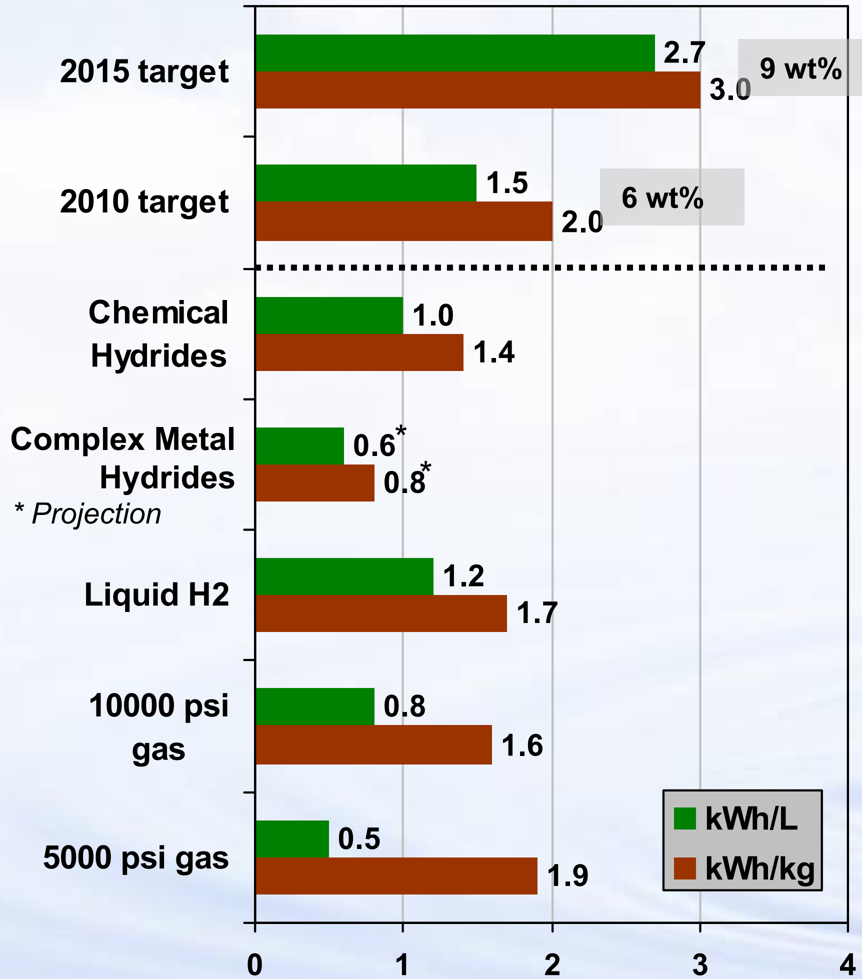


Portfolio stresses longer-term solutions but continues some R&D on viable options for the transition phase

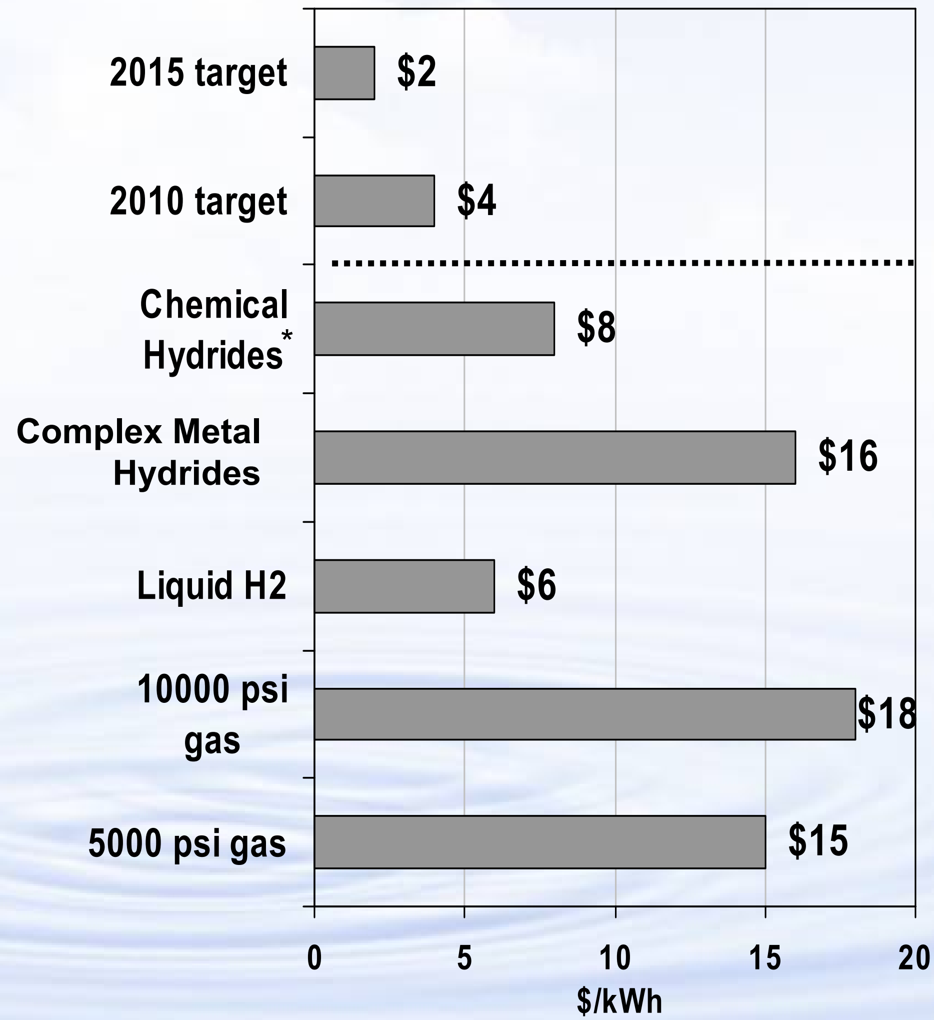
Status Relative to Targets

No current hydrogen storage technology meets the targets.

Volumetric & Gravimetric Energy Capacity

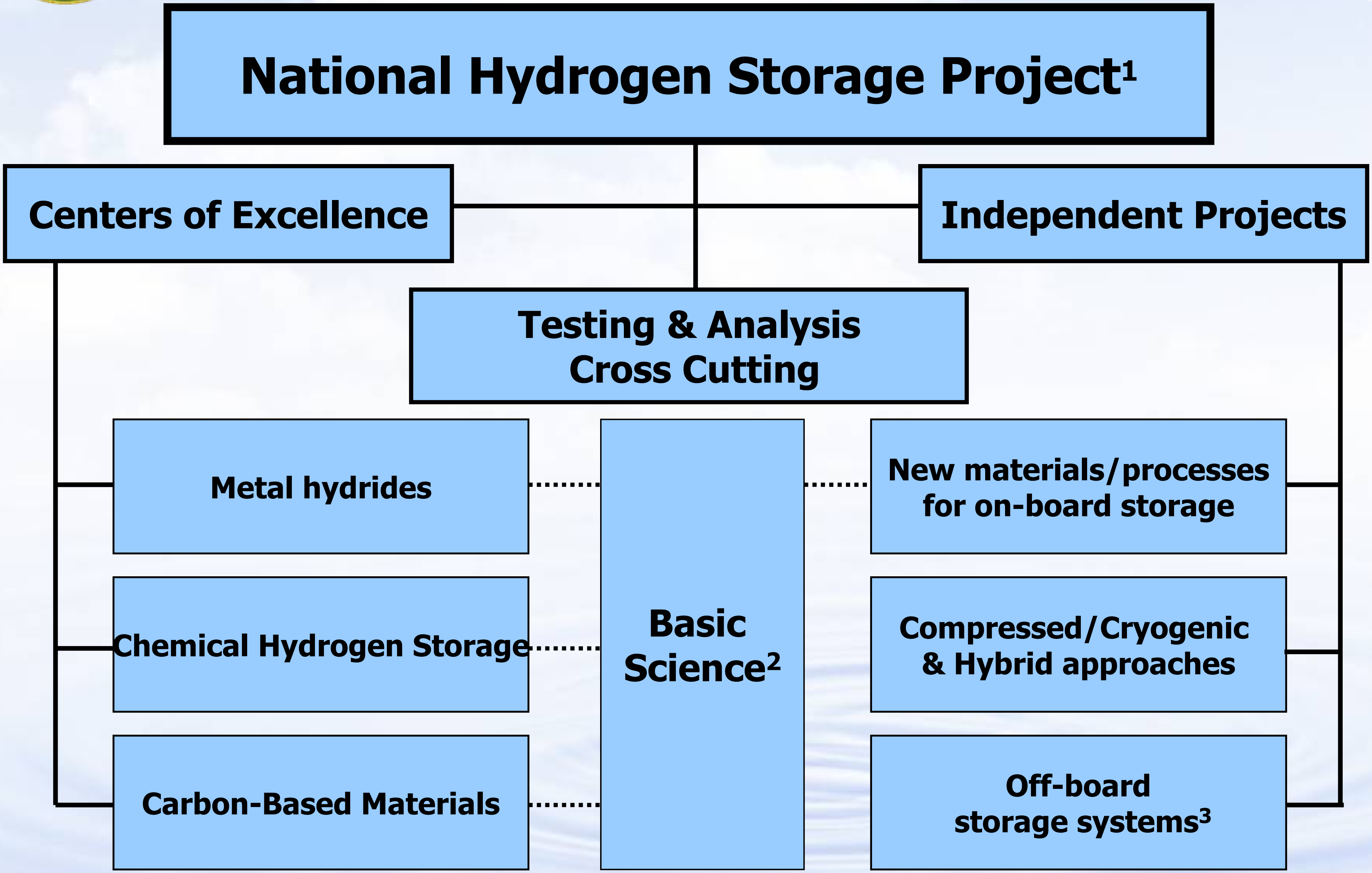


System Cost, $/kWh



Estimates from developers- to be continuously updated

* *Regeneration costs excluded*



1. Coordinated by DOE Energy Efficiency and Renewable Energy, Office of Hydrogen, Fuel Cells and Infrastructure Technologies
2. Basic science for hydrogen storage conducted through DOE Office of Science, Basic Energy Sciences
3. Coordinated with Delivery program element

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

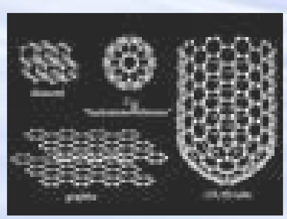
Federal Lab Partners:
Lawrence Livermore
NIST
Oak Ridge

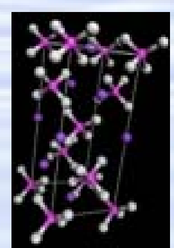
Chemical Hydrogen Center

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
Lawrence Livermore
Quantum
Argonne Nat'l Lab & TIAX LLC
SwRI

Continuum of Knowledge Transfer Across Stages of Development

Basic Research

Use theory & fundamental experimentation to generate knowledge:

- Fundamental property & transport phenomena
- Novel material structures, effect of morphology.
- Understand reaction mechanisms

Applied Research & Development

Use theory & experimentation to design & develop high-performance materials

- Leverage knowledge from basic research, develop new materials
- Optimization of materials and testing to improve performance
- Use engineering science to design system packaging & balance of plant components

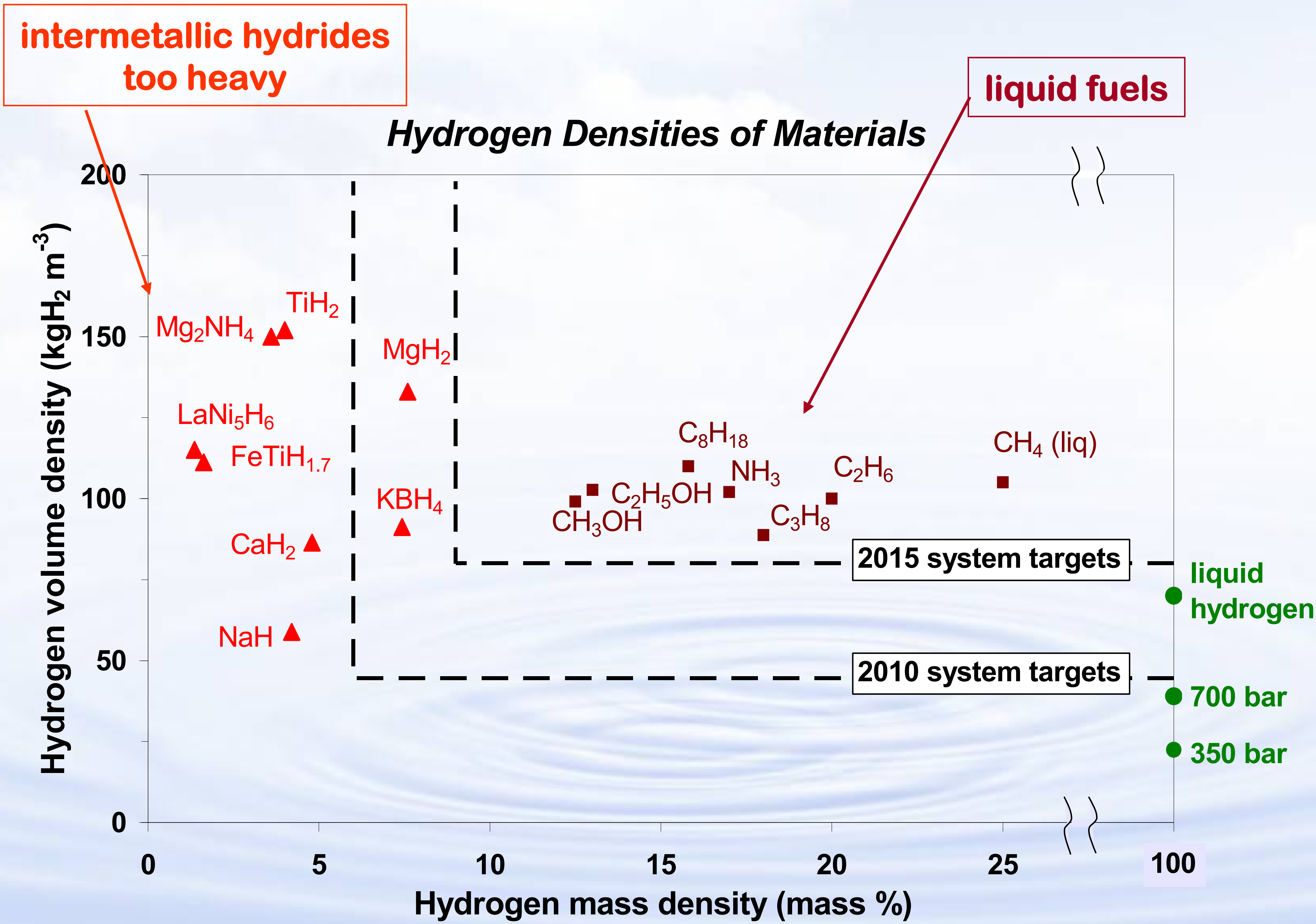
Technology Validation & Demonstration

Test Systems in Real World Conditions

- Gain knowledge on integration with power plant with fuel delivery infrastructure
- Apply lessons learned back to R&D

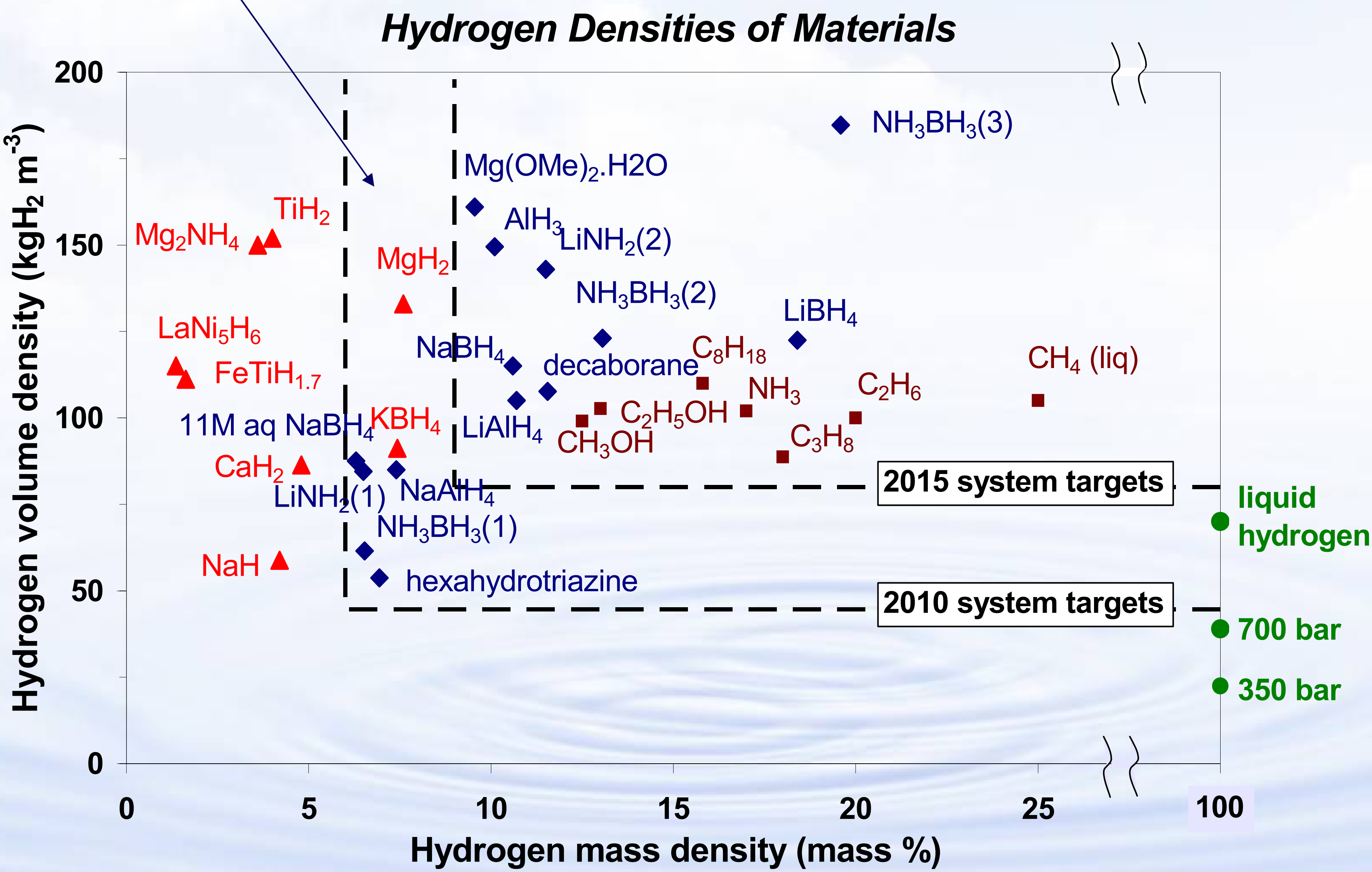
Basic Science for Hydrogen Storage

Basic material properties are a key issue in hydrogen storage.



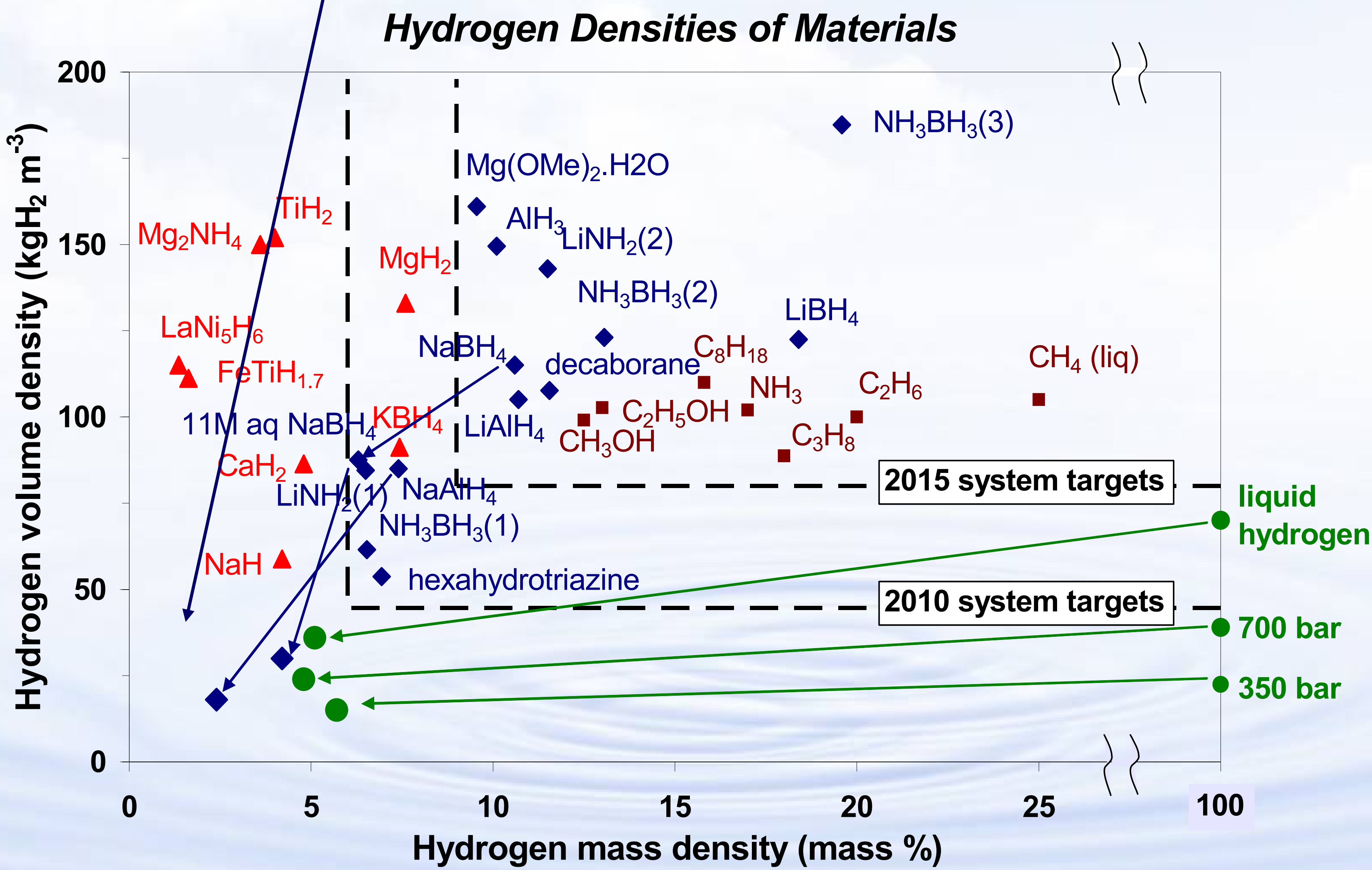
Program focus is on high energy density materials.

Some of the materials under study in CoE's



Storage system adds weight and volume

No current material meets system requirements



Need to determine & tune material properties

Other material property issues include thermodynamic properties.

For reversible systems, equilibrium between gas and solid given by:

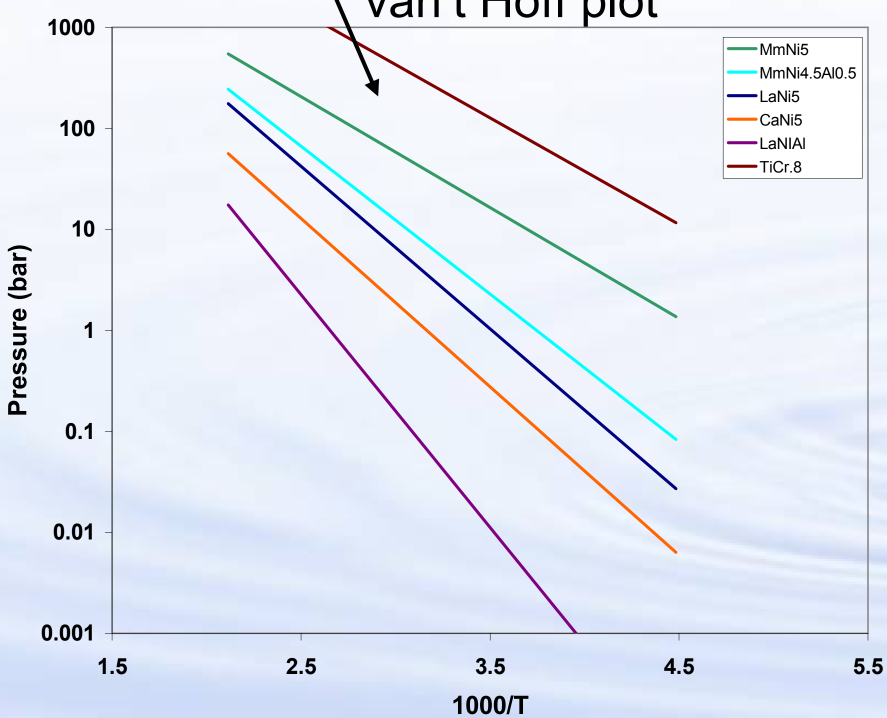
$$P = \exp(-\Delta H/RT + \Delta S/R)$$

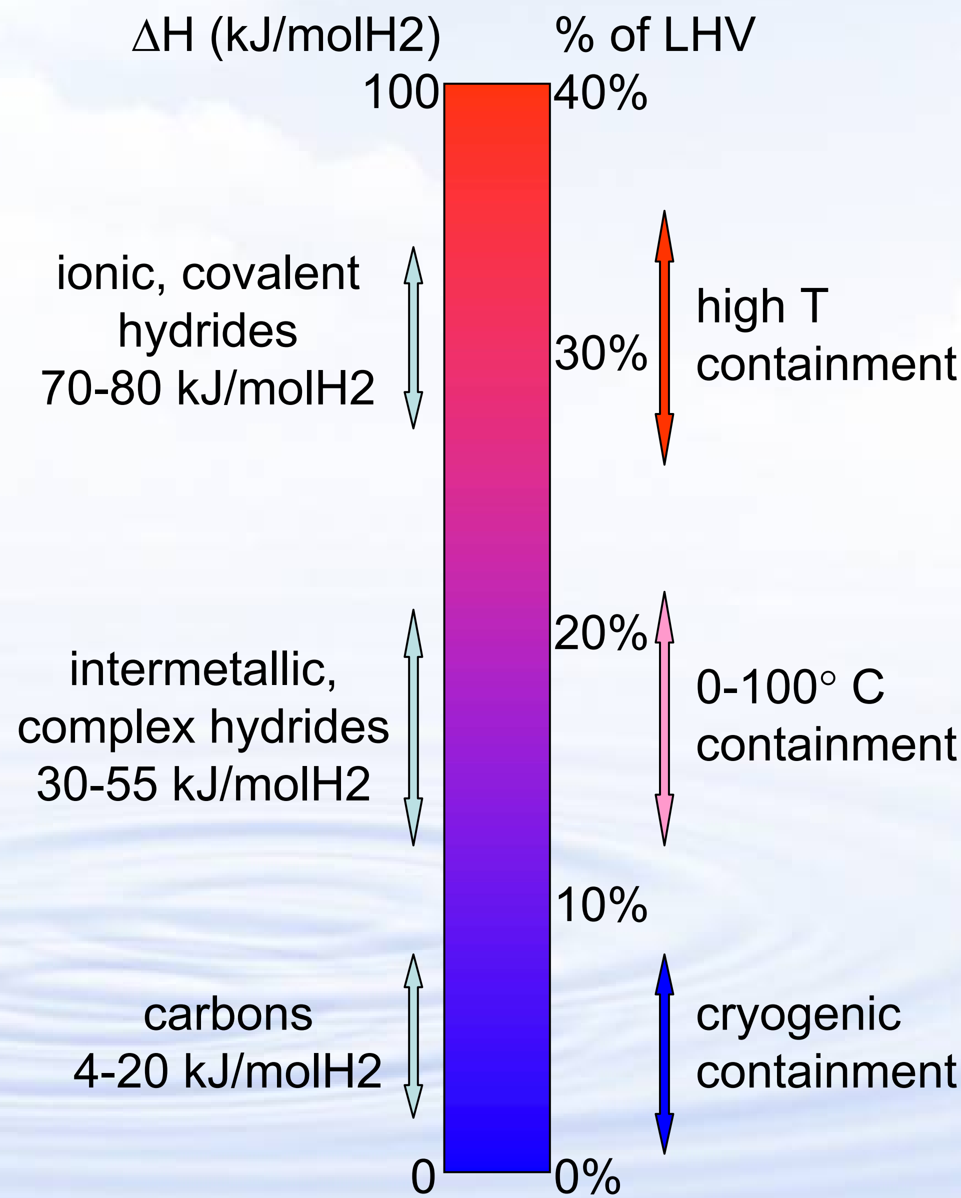
or $\ln P = -\Delta H/RT + \ln P_{Tinf}$

ΔH=enthalpy (kJ/mol H_2),

$$d(\ln P)/d(1/T) = \Delta H/R$$

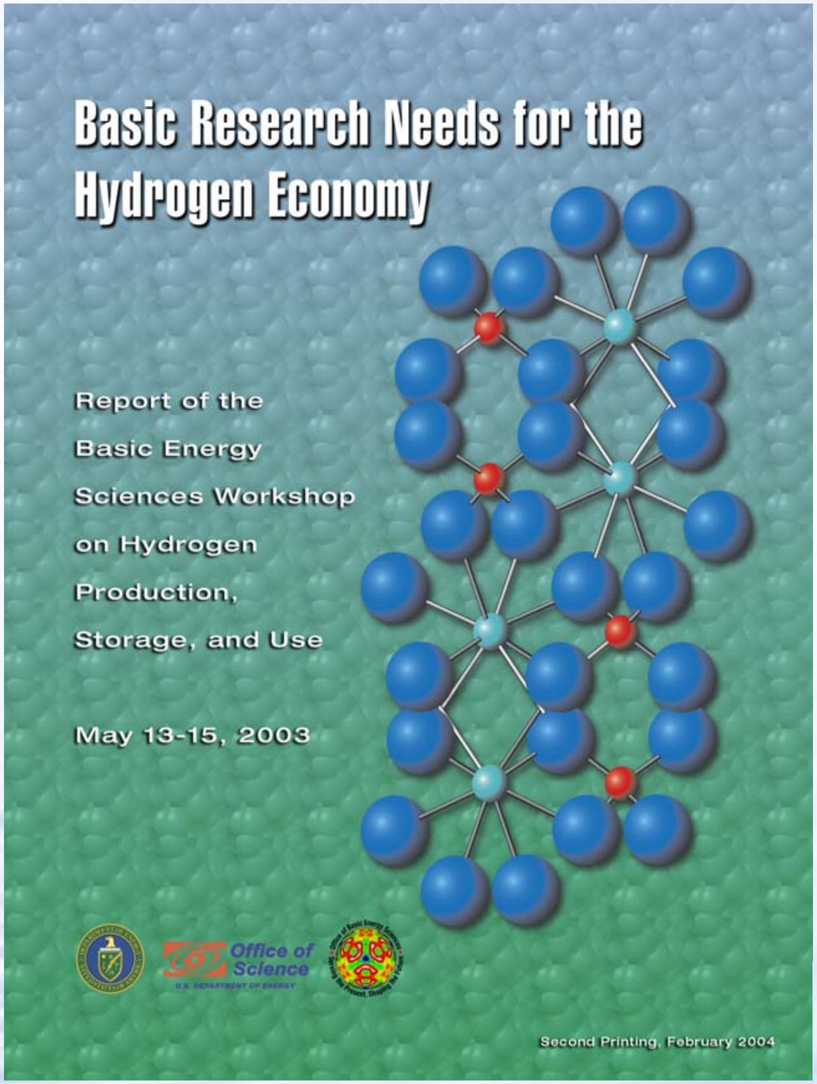
van't Hoff plot





BES workshop was held to identify basic research needs.

- Understanding the fundamental factors governing material behavior
- Applying these principles to modify material performance
- Identifying new materials and new classes of materials
- Designing of new materials at the nanoscale
- Theory, modeling and simulation of materials and molecular processes



Workshop laid foundation for 2005 BES solicitation.

- 227 full proposals were received
- Five technical focus areas:
  - Novel materials for hydrogen storage (50 proposals)
  - Membranes for separation, purification and ion transport (52 proposals)
  - Design of catalysts at the nanoscale (56 proposals)
  - Solar hydrogen production (49 proposals)
  - Bio-inspired materials and processes (20 proposals)

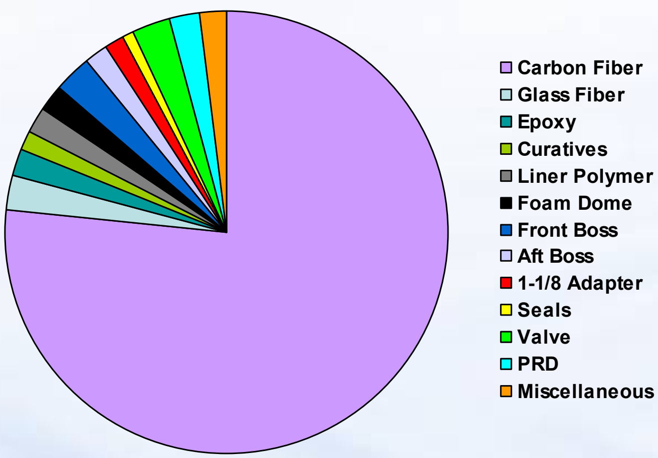
Stay tuned for further announcements!

Tanks- Accomplishments & Status

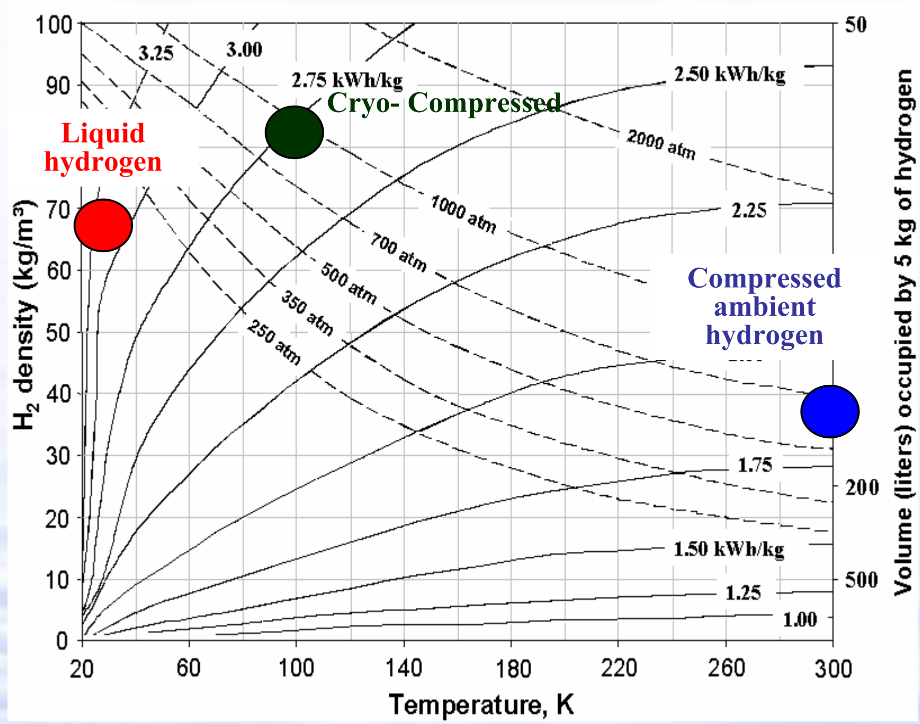
Tanks: Performance close to targets - Next steps are cost and hybrid approaches.

		Specific Energy	Energy Density	Cost
	2015 Targets (2010)	3.0 kwh/kg (2.0)	2.7 kwh/L (1.5)	$2/kWh (4)
Status* (Quantum)	5,000 psi System	1.9 kwh/kg	0.5 kwh/L	$15/kWh
	10,000 psi System	1.6 kwh/kg	0.8 kwh/L	$18/kWh

Primary driver is material cost
40 - 80% is carbon fiber cost



Future focus: Cost reduction, advanced concepts, conformability



Density improvements possible with cryo-compressed H

Aceves, et al, LLNL

* 5 kg storage using one tank; volume of 500,000 tanks/year

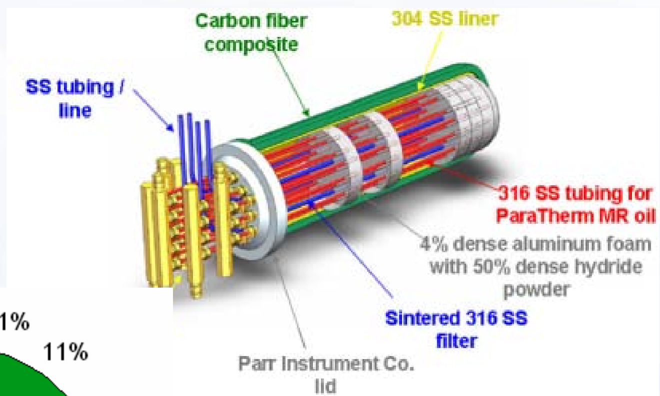
Storage Accomplishments- Metal Hydrides

System Engineering:

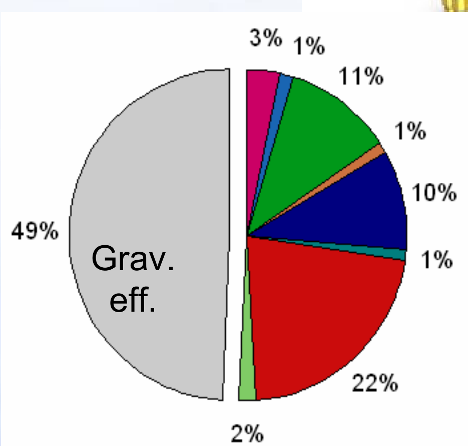
- Preliminary 1-kg hydrogen system prototype developed ***(Anton, et al, UTRC)***
- With composite vessel, ~50% of system is balance of plant

Materials Development:

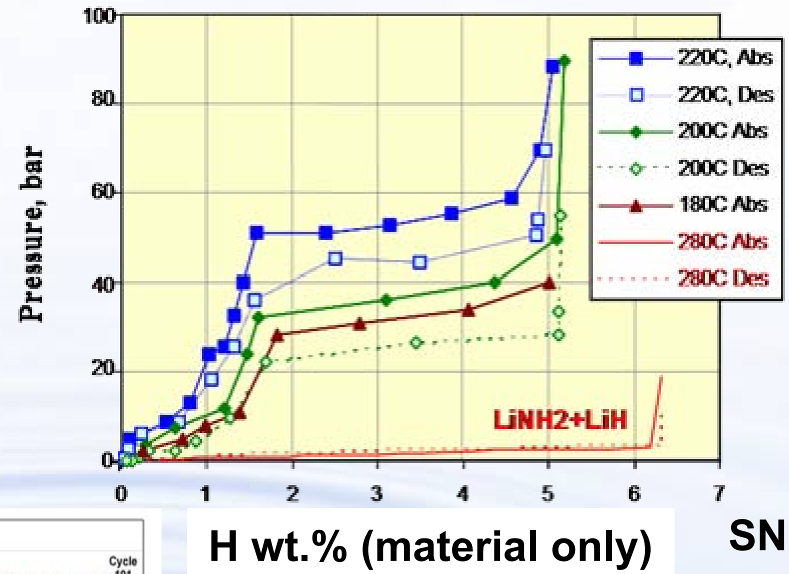
- Mg modified Li-amides demonstrate 5 wt% materials-based capacity, reversible with potential up to 10 wt% ***(Luo, Wang, et al, SNL)***
- Absorption demonstrated down to 180C with Mg substitution
- Over 100 cycles demonstrated for Li/Mg amide system ***(Luo, Gross, et al, SNL***



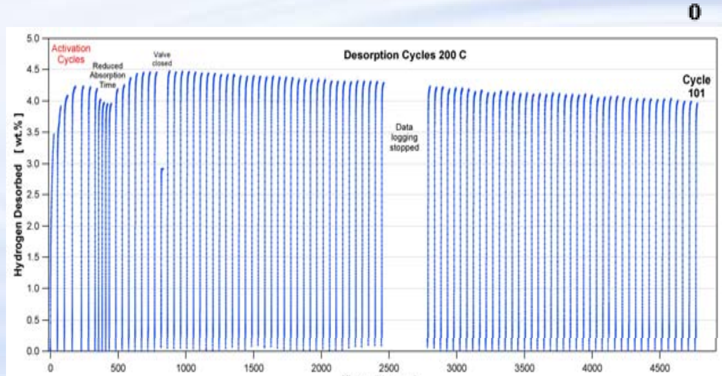
UTRC



660 Wh / kg **530 Wh / L**



SNL



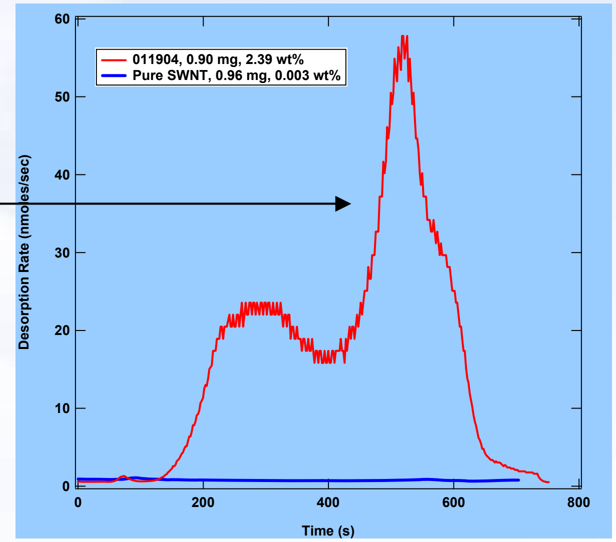
← 0.005 wt% loss/cycle

SNL

Storage Accomplishments- Carbon Materials

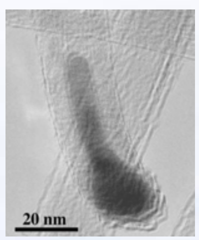
- Doped single-wall nanotubes (SWNTs) synthesized and capacity measured to be ~2.5 - 3 wt.% hydrogen storage

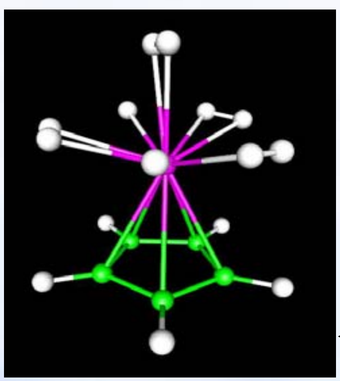
- Binding energies calculated and optimum compounds theoretically predicted for potential storage materials



H_2 Desorption

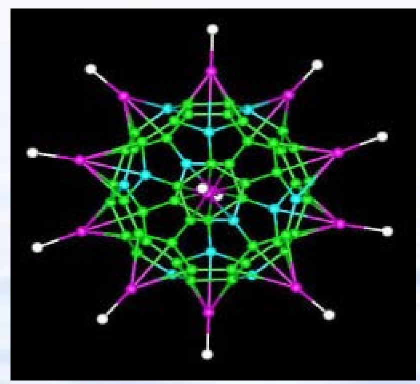
Iron in nanotube

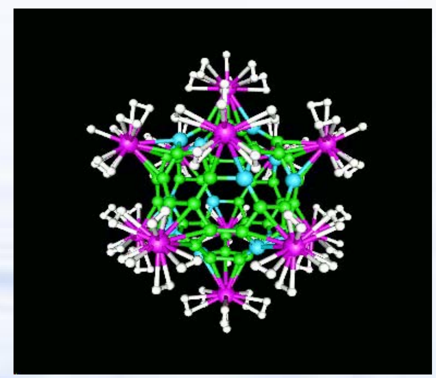




$Cp[ScH_2(H_2)_4]$

0.23 eV





$$C_{48}B_{12}[ScH]_{12} \underset{}{\overset{60H_2}{\rightleftarrows}} C_{48}B_{12}[ScH(H_2)_5]_{12}$$

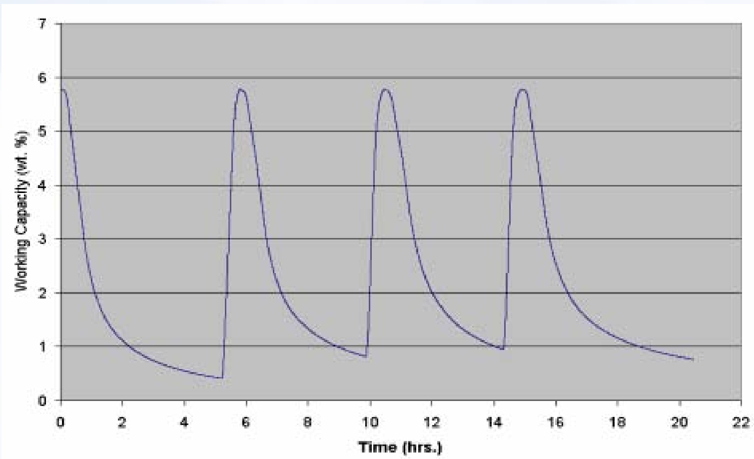
Potential for 8.8 wt%

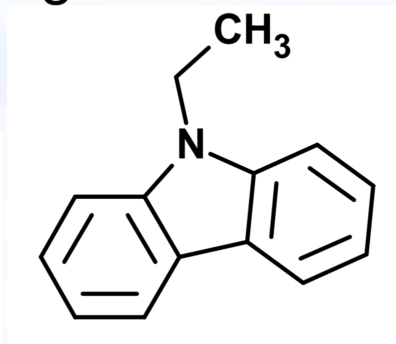
Heben, Dillon, et al
NREL, Golden, CO

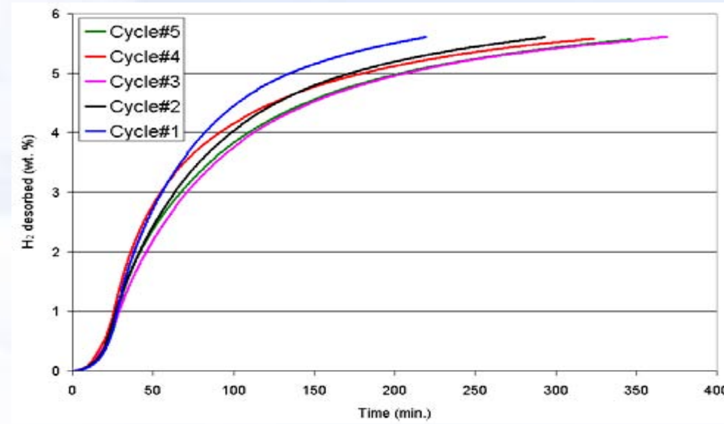
Storage Accomplishments- Chemical Hydrides

- Identified chemical hydride with 5.5 wt% materials-based H_2 storage capacity

N-ethylcarbazole



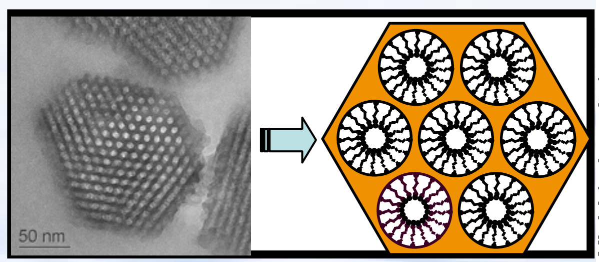




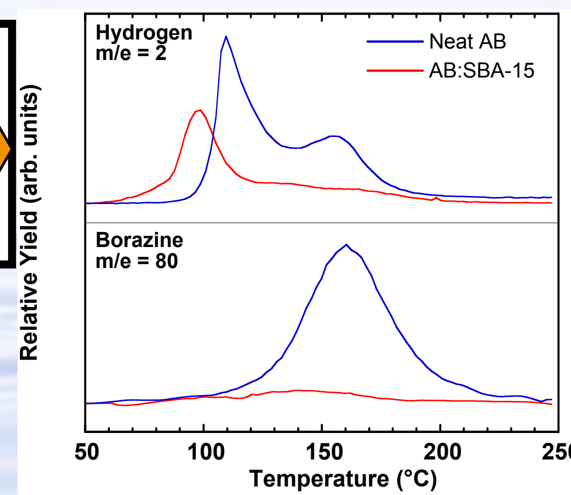
Cooper, Pez, et al, Air Products

- Demonstrated several cycles
- 40 catalysts screened for dehydrogenation

- Mesoporous scaffolds internally coated with ammonia borane show hydrogen release at < 100 C and reduce borazine formation

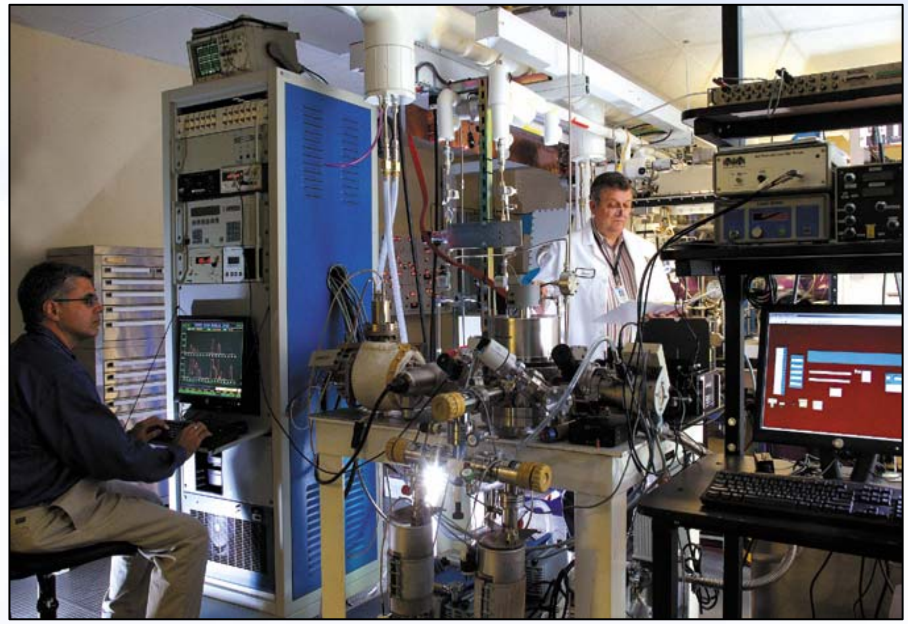


Autrey, et al, PNNL



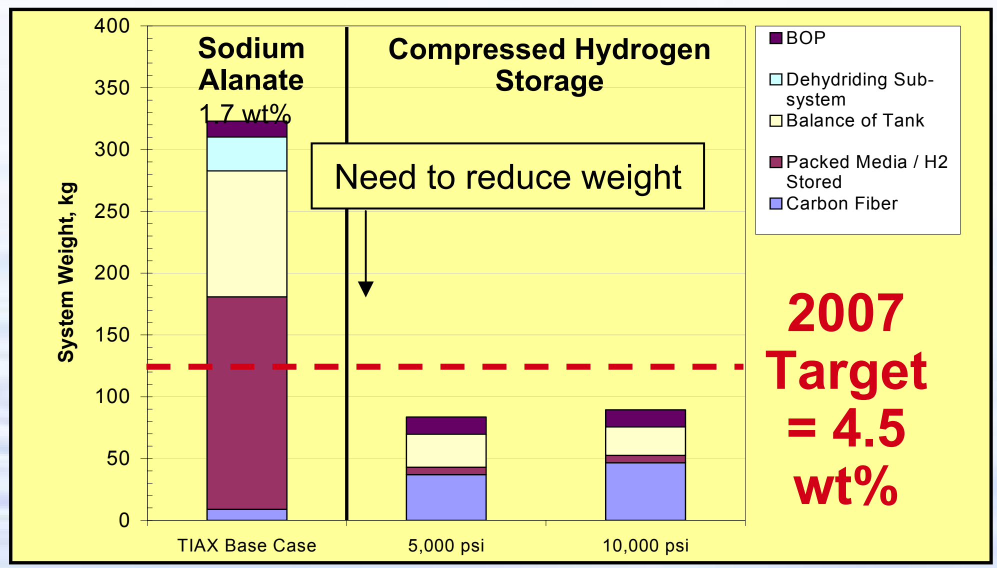
Independent Testing and Analysis

- Standardized Test Facility
  - Independent laboratory, SwRI
  - Construction complete
  - Test protocols developed
  - Website planned
  - Validation underway (double-blind testing)



SwRI

- Storage Systems Analyses
  - Storage Systems Analysis Working Group formed (March, ’05)
  - Need for independent analyses: Performance, cost, life cycle energy & environmental impact, toxicity, safety
  - Breakdown of system into components (TIAX, ANL, Quantum, UTRC, Safe H2, Millennium Cell)



TIAX

Key Activities and Outputs (2005-2006)

IPHE Hydrogen Storage Technology Conference
June 20-22, 2005, Barga, Lucca, Italy

Italy

U.S. DOE

European Commission

Russian Federation

Key Organizers:
P. Garibaldi, S. Malyshenko, M. Steen, G. Sandrock, M. Conte, C. Filiou, S. Satyapal

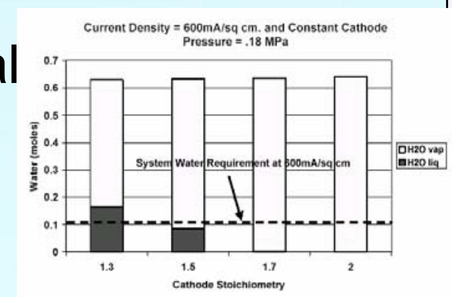
- Forum for Technical experts in hydrogen storage worldwide
- Track global progress- inventory of projects & expertise
- Objectives: Promote leveraging of global R&D
  - Identify and reduce duplication
  - Create and strengthen partnerships
  - Initiate process, identifying clear guidelines for IPHE projects
  - Gather feedback from global technical community on issues to be addressed by IPHE
  - Accelerate collaborative research projects
  - Recommendations to IPHE Committees

Limited Attendance: www.iphe.net or http://www.engconfintl.org/5ar.html

Key Activities and Outputs (2005-2006)

FreedomCAR & Fuel Partnership

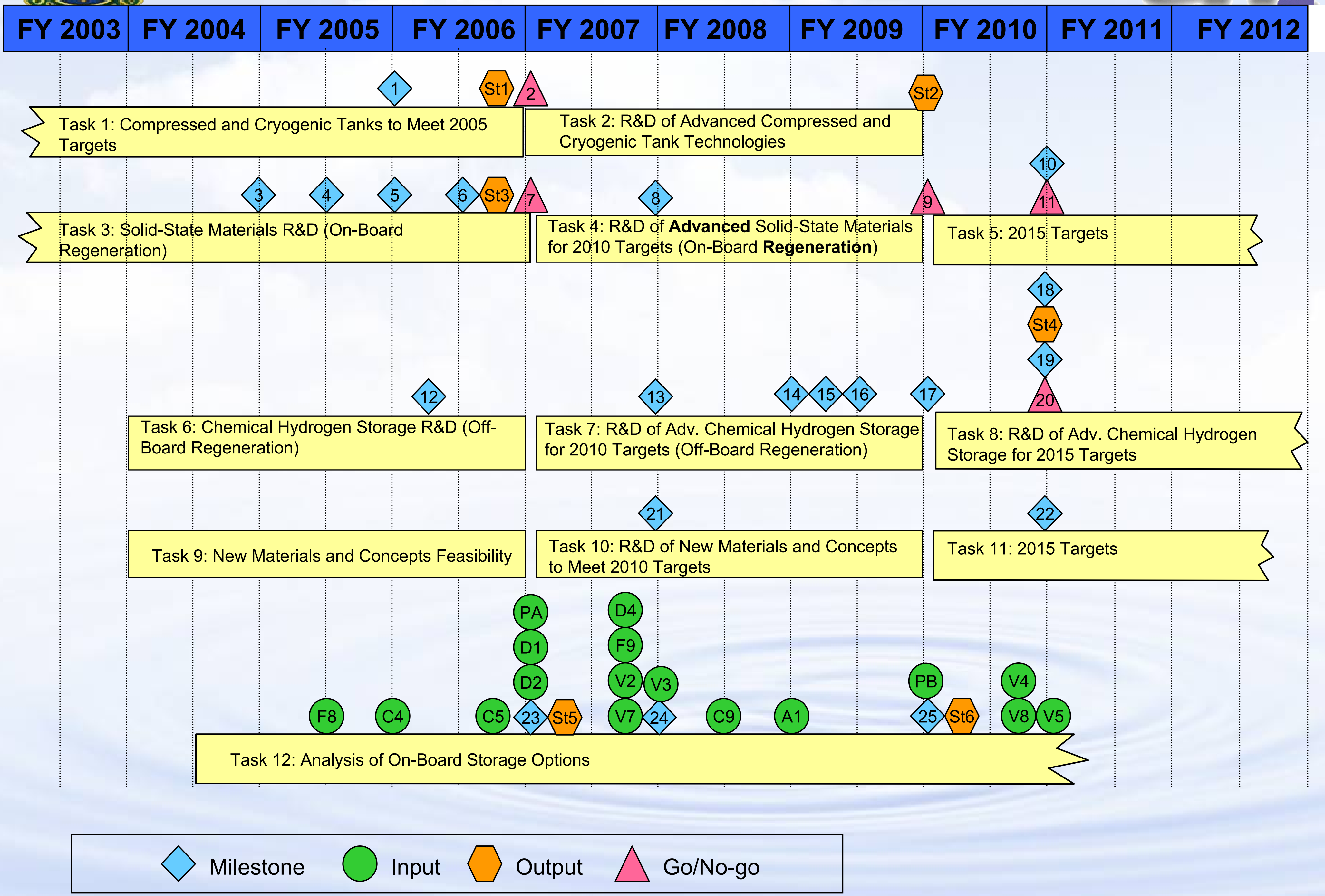
- Water Availability Model → Help guide chemical hydrogen storage researchers



- Position Paper on Ammonia → Draft for public comment, June 2005
- Review Targets & Update → June-August 2005
- Purity Specification Guidelines
  - Input to storage systems
  - Output from storage systems

→ Tolerance of storage materials to various contaminants
Coordination with Fuel Cell, Production & Delivery Program Elements

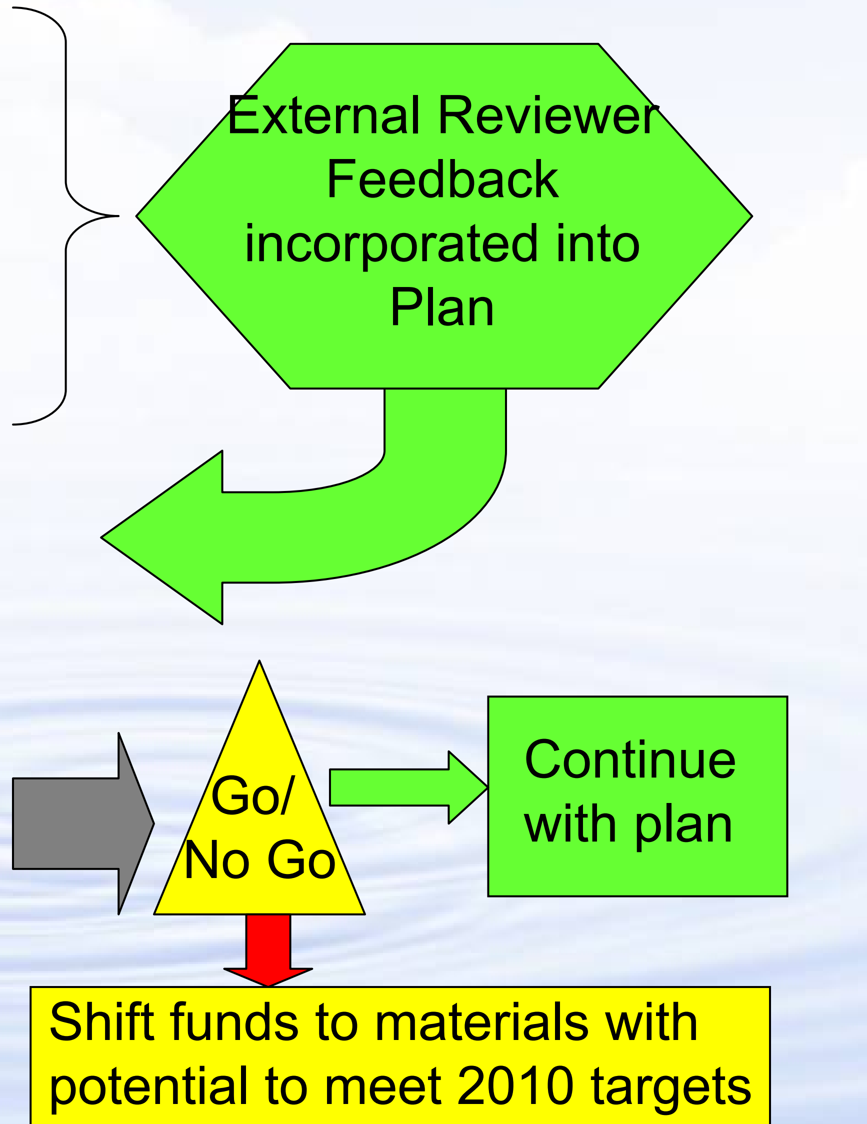
RD&D Plan- Tasks, Milestones



Go/No-Go Decision on Carbon Nanotubes (4Q FY 06)

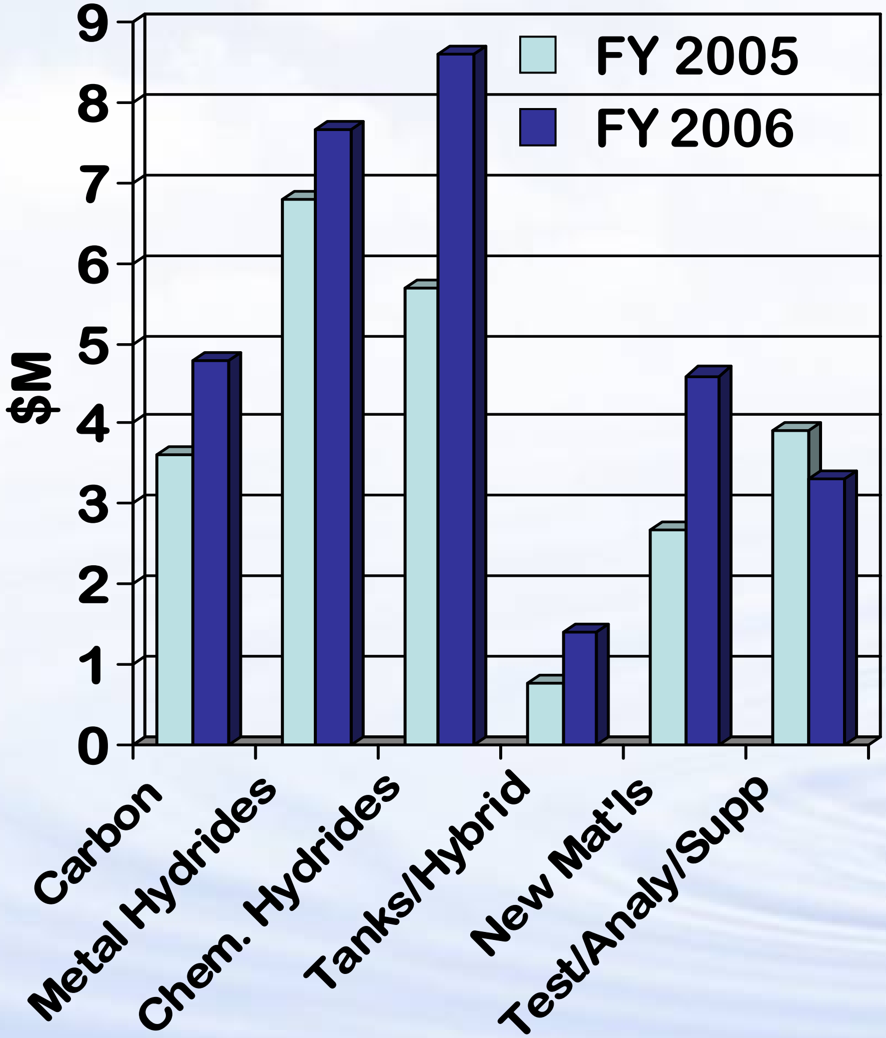
Decision Planning & Implementation

- **Measurement Technique Validation**
  - ✓Verify storage capacity measurement with 2 different techniques
  - ✓Verify accuracy with standards
  - ✓On-site peer review to inspect & verify measurement techniques (Jan. '04)
- **Interim Milestone:**
  - ✓Demonstrate 3 wt % (materials-based storage capacity - Aug. '04)
- **Interim Milestone:**
  - o Demonstrate 4 wt % (materials-based storage capacity)
- **Milestone:**
  - o Reproducibly demonstrate 4 wt% in external laboratory (4Q FY 2005)
- **Go/no go Point:**
  - o Reproducibly demonstrate 6 wt% (materials-based storage capacity) in *external laboratory* (4Q FY 2006)



Budget: FY 2005 vs. FY 2006 Request

FY2006 Budget Request = $29.9M
FY2005 Appropriation = $24.4M



- **Emphasis:**
  - Continue Centers of Excellence and new materials projects to focus on 2010 hydrogen storage goals of 2.0 kWh/kg, 1.5 kWh/liter, $4/kWh
  - Independent Testing & Analysis

- **Budget Distribution:**

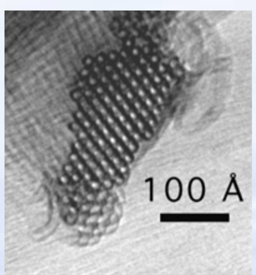
Centers of Excellence	$16.7M
Independent Projects & Support	$13.2M
Total	$29.9M

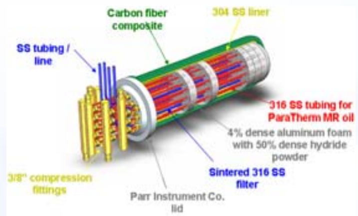
Key Milestones

Complete construction of materials test facility (4Q, 2004)

2005

Demonstrate 4 wt% storage capacity on carbon nanotubes (4Q, 2005)



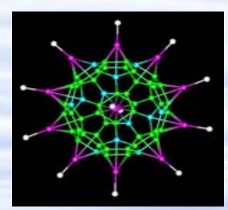


Complete prototype complex metal hydride system (2Q, 2006)

2006

Go/no go based on 6 wt% storage capacity on carbon nanotubes (4Q, 2006)

2007



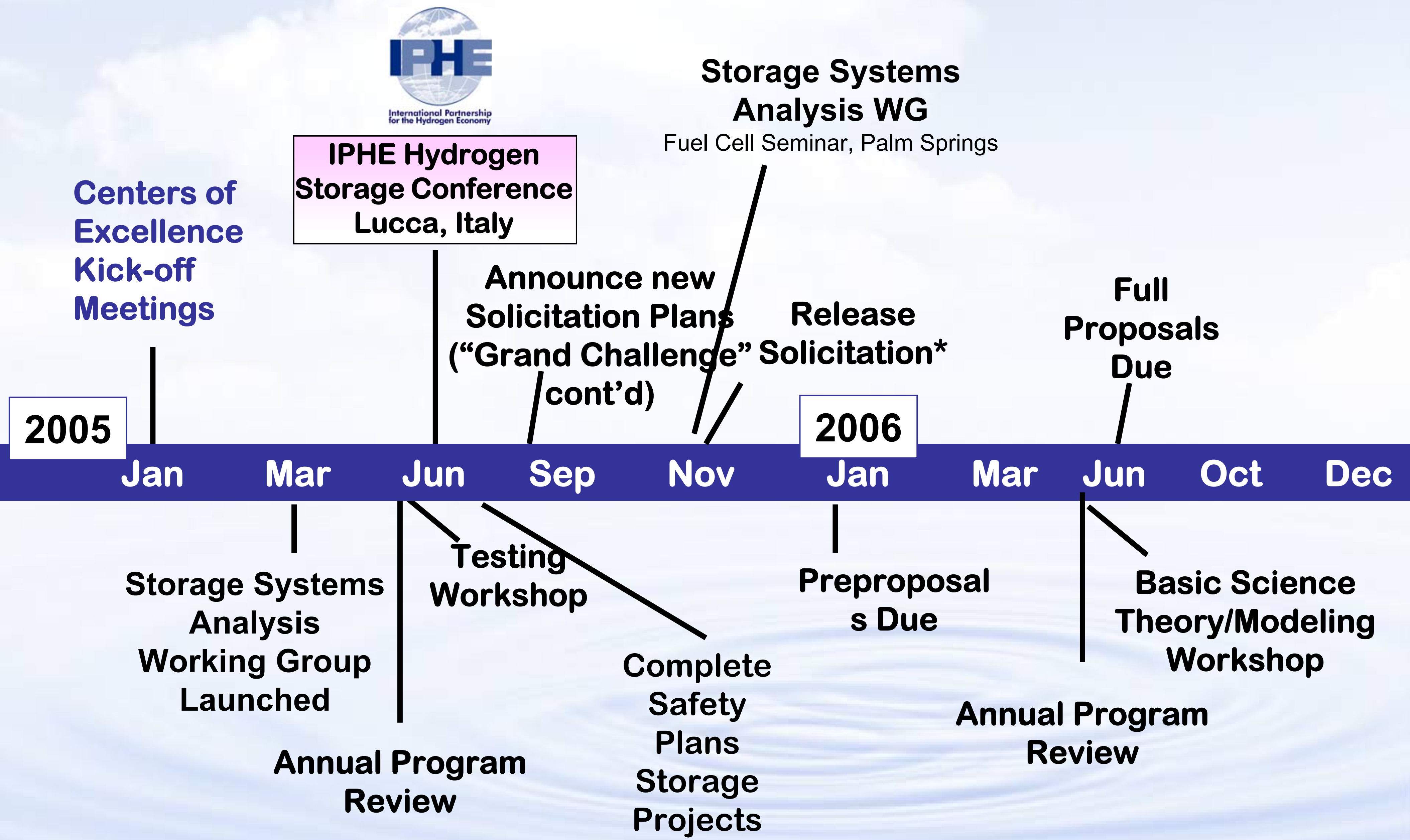
Down-select reversible metal hydrides (4Q, 2007)

2008

Down-select regeneration processes for chemical hydrides (4Q, 2007)

Down-select new materials / concepts (4Q, 2006)

Hydrogen Storage – Future Plans



*Subject to appropriations

For More Information, Contact:

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- **Carole J. Read**: *Metal Hydrides, Metal Hydride Center of Excellence*
  - Phone 202-586-3152; *carole.read@ee.doe.gov*
- **John Petrovic:** New concepts and materials, *Laboratory Fellow, Change of Station assignment from LANL*
  - Phone 202 586-8058; john.petrovic@ee.doe.gov
- New Hire: *Materials science/engineering expertise junior/mid-level scientist/engineer- to be posted*

- **Sunita Satyapal**: Hydrogen *Storage Team Leader, Carbon Center of Excellence, Tanks, Analysis, IPHE activities*
  - Phone 202-586-2336; *sunita.satyapal@ee.doe.gov*

(Basic Science Contact: Harriet Kung, harriet.kung@science.doe.gov)

www.hydrogen.energy.gov