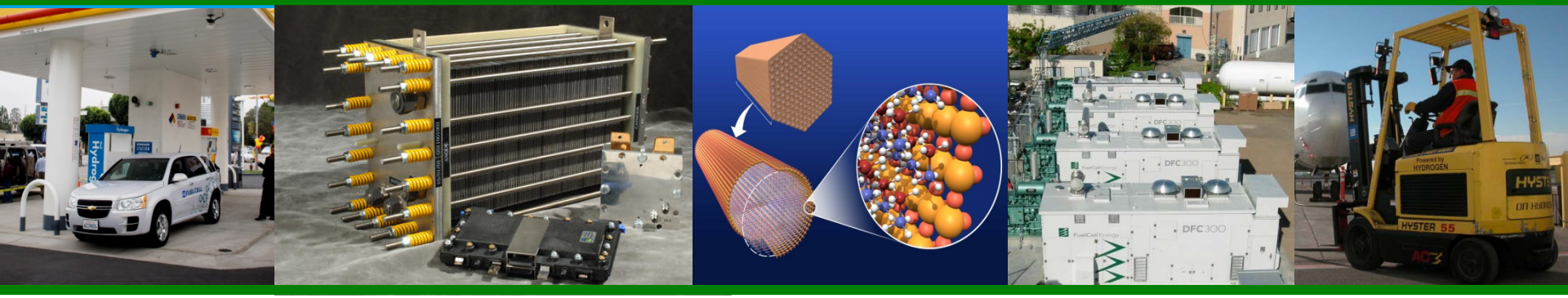
U.S. DEPARTMENT OF ENERGY



Hydrogen Storage Program Area
-Plenary Presentation-

Ned T. Stetson

Fuel Cell Technologies Office

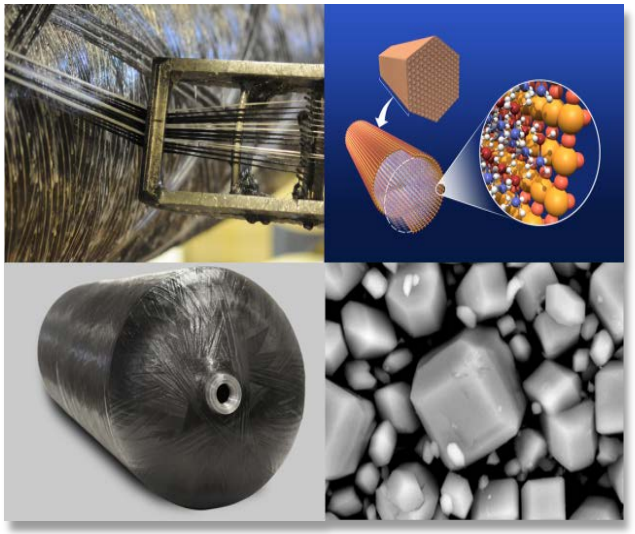
2016 Annual Merit Review and Peer Evaluation Meeting

June 6 - 10, 2016

Goals and Objectives

Objectives

- By 2020, develop onboard vehicle H_2 storage systems achieving **1.8 kWh/kg** (5.5 wt% H_2) and **1.3 kWh/L** (40 g H_2/L) at **$10/kWh** ($333/kg $H_{2\ stored}$) or less.
- By 2020, demonstrate H_2 storage systems in MHE applications achieving **1.7 kWh/L** (50 gH_2/L); ability to recharge with 2 kg of H_2 within 2.8 minutes at **$15/kWh** ($500/kg $H_{2\ stored}$) or less.
- Ultimate targets: to develop onboard H_2 storage systems achieving **2.5 kWh/kg** (7.5 wt.% H_2) and **2.3 kWh/L** (70 g H_2/L) at **$8/kWh** ($266/kg $H_{2\ stored}$) or less.
- Other specific objectives are in the Hydrogen Storage Section of the MYRD&D Plan.





GOAL: Develop advanced hydrogen storage technologies to enable successful commercialization of hydrogen fuel cell products

Hydrogen Storage Team - Strategy and Barriers

Dual approach

Hydrogen Storage

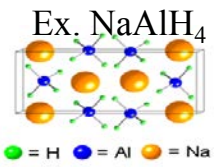
- Near-Term Approach
- Longer-Term Approach

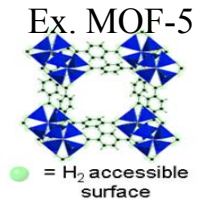
Technology Focus

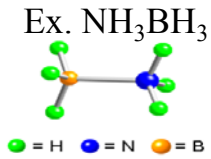
- 700 bar Compressed
- Cold / Cryo-Compressed
- Metal Hydrides
- Sorbents
- Chemical H_2 Storage











Barriers and R&D Focus

- Lower Cost Carbon Fiber
- Improved Composites
- Conformable designs
- Lower Cost BOP

- System Engineering
- Advanced Insulation
- Improved Dormancy
- Composite Development

- Higher Material Capacity
- System Cost
- Fill Time
- Onboard Efficiency

- Higher Material Capacity
- System Cost
- Dormancy
- WTP Efficiency

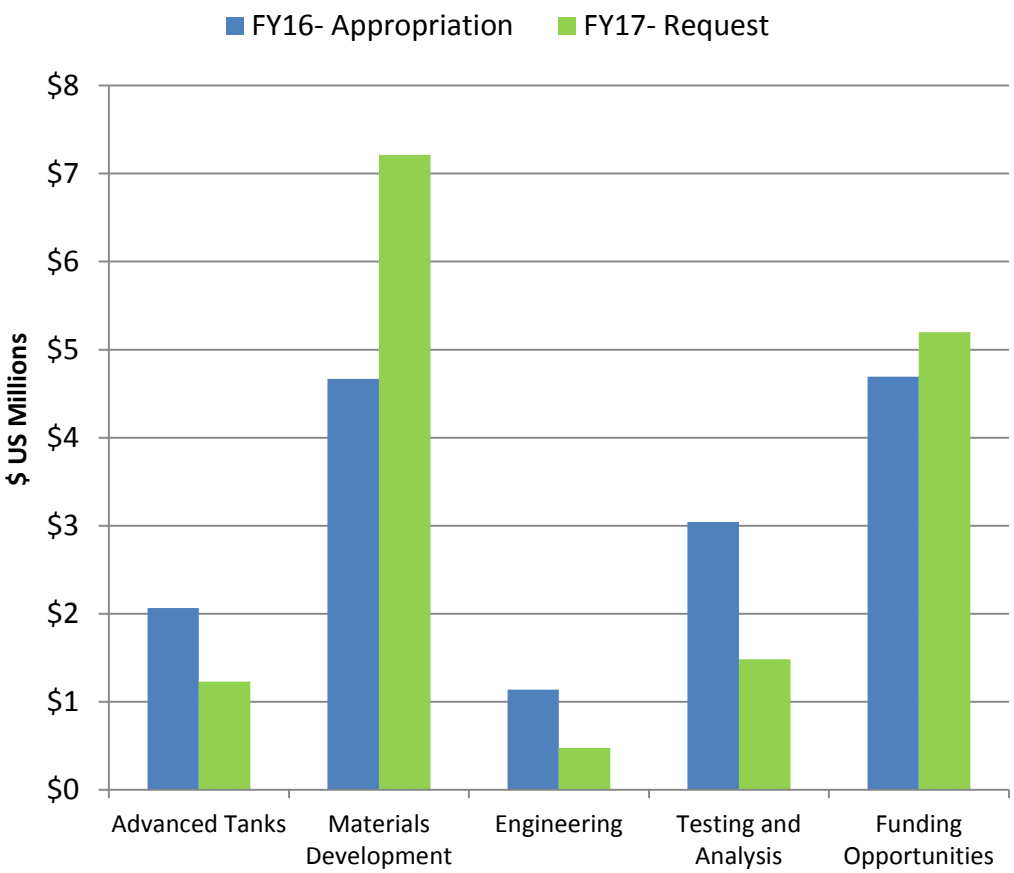
- Lower Cost Off-board Regen
- System Cost
- Gravimetric Density

Objective: Achieve a driving range >300 miles for full span of light-duty vehicles, while meeting packaging, cost, safety, & performance requirements

Budget

FY 2016 Appropriation = $15.6M

FY 2017 Request = $15.6M



EMPHASIS

- Close coordination with EERE Offices on carbon fiber composites, including AMO, VTO and BETO
- Focus on cost reduction for high pressure tanks
- Increase materials development efforts through national lab-led consortium, HyMARC, and materials characterization and validation capabilities
- Portfolio is balanced between mid- and long term

Steady budget for several consecutive years, annual FOAs to initiate new projects in target technology areas

Current Status of H_2 Storage Technologies

Storage Targets	Gravimetric kWh/kg (kg H_2/kg system)	Volumetric kWh/L (kg H_2/L system)	Costs $/kWh ($/kg H_2)
2020	1.8 (0.055)	1.3 (0.040)	$10 ($333)
Ultimate	2.5 (0.075)	2.3 (0.070)	$8 ($266)

Full set of comprehensive hydrogen storage targets can be found in the Program's Multi-year Research, Development and Demonstration Plan: http://energy.gov/sites/prod/files/2015/05/f22/fcto_myrdd_storage.pdf

Projected H_2 Storage System Performance (5.6 kg H_2 usable)	Gravimetric kWh/kg (kg H_2/kg system)	Volumetric kWh/L (kg H_2/L system)	Costs* $/kWh ($/kg H_2)
700 bar compressed (Type IV, Single Tank)	1.4 (0.044)	0.8 (0.024)	$15 ($500)
Metal Hydride ($NaAlH_4$/Ti)	0.4 (0.012)	0.4 (0.012)	$43 ($1,432)
Sorbent (MOF-5, 100 bar, MATI, LN2 cooling)	1.3 (0.04)	0.7 (0.020)	$16 ($533)
Chemical Hydrogen Storage (AB-50 wt.%)	1.4 (0.043)	1.3 (0.040)	$17 ($566)

- 700 bar compressed H_2 system projections from ANL / SA
- Materials-based system projections from Hydrogen Storage Engineering Center of Excellence (5/2015)

* Projected at 500,000 units / year

Physical Storage

Accomplishments - Project Highlights

Low-cost CF precursors [ORNL/VT]

- Approach: Melt-spinning process to produce PAN/comonomer fiber for use as precursor for high-strength CF production
- Goal: ~30% lower cost CF than with conventional PAN precursor fibers
- **Down-selected water/plasticizer combinations for PAN/VA formulations and demonstrated spinning of >100 filament tows of length >10m**



Modified extruder feed



Melt-spun PAN/MA fiber

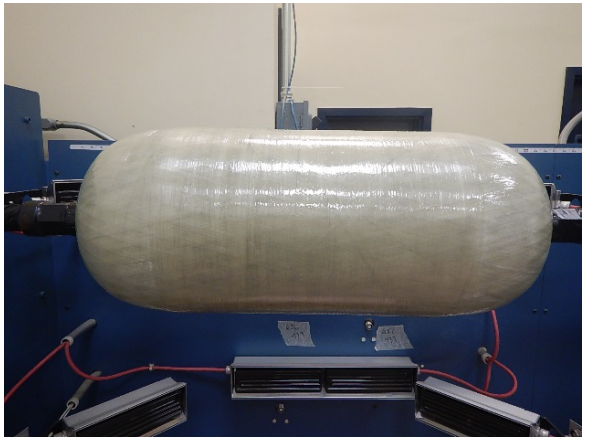
ST093

Low-cost alternative fibers to CF [PPG/Hexagon Lincoln/PNNL]

- Approach: Ultra-high strength fiber glass
- Goal: New fiber glass with tensile strength exceeding Toray T700 CF at ~50% of cost
- Demonstrated pilot scale high temperature glass fiber manufacturing process and produced 1200 lb of fiber glass
- High strength fiber tanks outperformed the reference fiber tanks on burst pressure and cyclic pressure tests.
- **One high strength fiber with sizing A significantly outperformed on stress rupture test.**



Batch melting process



Vessel winding

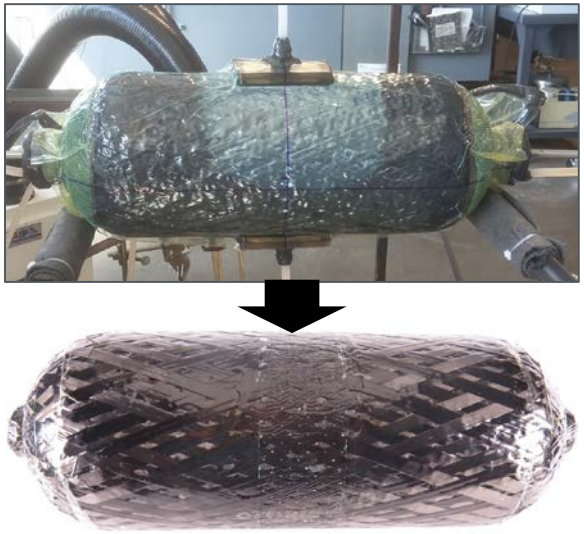
ST115

Reducing cost of composites for use in H_2 storage vessels

Accomplishments - Project Highlights

Alternative resin and manufacturing [Materia/MSU/Spencer Composites]

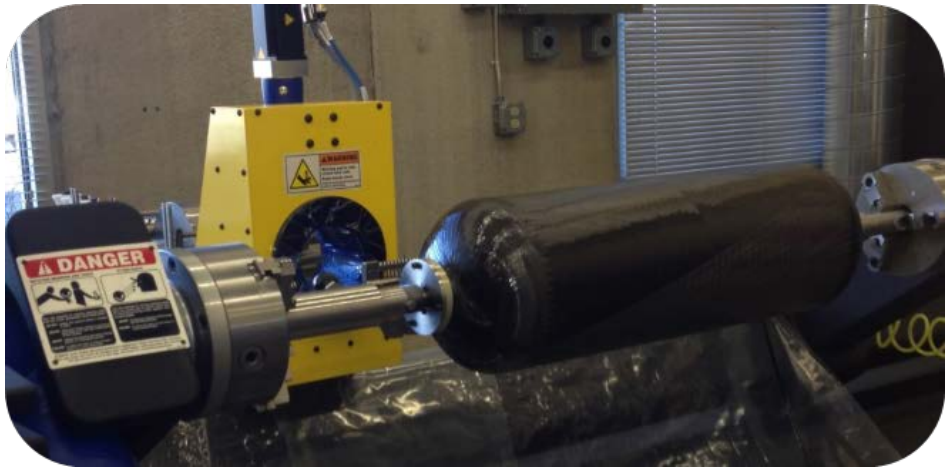
- Approach: low-viscosity, high-toughness resin with VARTM manufacturing process
- Goal: 35% reduction in composite costs
- Optimized vacuum infusion process and winding pattern, achieved infusion of high quality, small COPV
- **Achieved burst pressure of 732 ksi compared to 693 ksi obtained from a wet wound epoxy resin tank.**



ST114

Optimized cost and performance of COPVs [CTD/ORNL/Adherent Tech.]

- Approach: Graded construction utilizing thick wall effect
- Goal: demonstrate potential for 10-25% lower cost through graded-construction approach
- Evaluated Panex 35 ™ as potential lower-cost candidate fiber to replace portion of Toray T700S
- **Updated Analysis: Cost reduction potential of 9-33%**



ST110

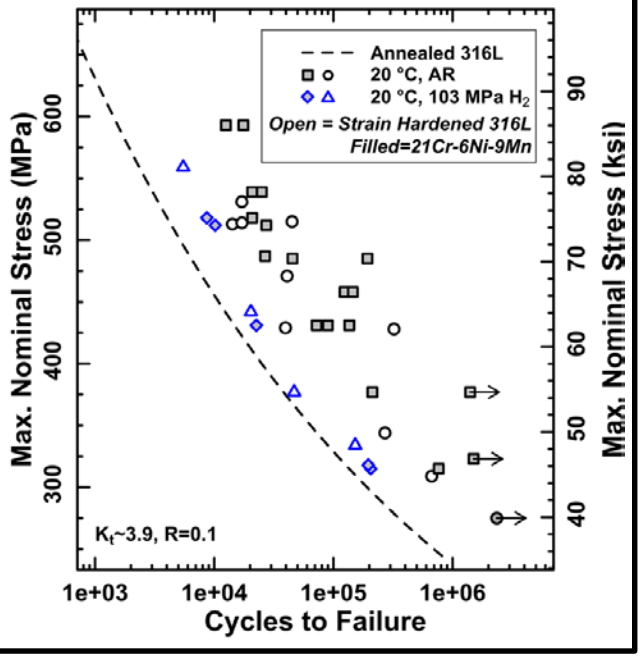
Reducing cost of H_2 storage vessels through alternative manufacturing

Accomplishments - Project Highlights

Alternative materials for BOP [SNL/Hy-Performance Materials]

- Approach: Screening based on fatigue stress and computational material design
- Goal: Reductions in BOP of up to 50% in weight and 35% in cost
- **Fatigue performance quantified for low-Ni austenitic stainless steel: 21Cr-6Ni-9Mn (XM-11).**

Fatigue life for both XM-11 and strain-hardened 316L exceeded annealed 316L baseline material's fatigue life.



ST113

Conformable 700 bar H_2 Storage Systems [CTE/HECR/UT]

- Approach: Develop a light weight, low cost over-braided, coiled pressure vessel for 700 bar H_2 storage
- Goal: Surpass DOE system targets for specific energy (3.7 kWh/kg) and cost (< $10/kWh)
- Achieves efficient onboard vehicle packaging through use of a shaped corrugated core over-braided with aramid fiber for strength
- **Selected resin for prototype vessel permeability testing**



Kevlar Overbraiding



Over-braided coiled vessels

ST126

Alternative materials for BOP and conformable designs

Accomplishments - Project Highlights

Cold-compressed H_2 storage [PNNL/Ford/Hexagon Lincoln/AOC/Toray]

- Approach: Synergistically consider pressure vessel and operating conditions (500 bar, 200 K)
- Goal: 30% reduction in system cost over 2013 baseline cost for 700 bar system
- Vinyl Ester and epoxy resin composites both show improved strength at 200 K
- **Lower-cost vinyl ester resin (XR-4079) able to match epoxy performance with 5-7% weight**

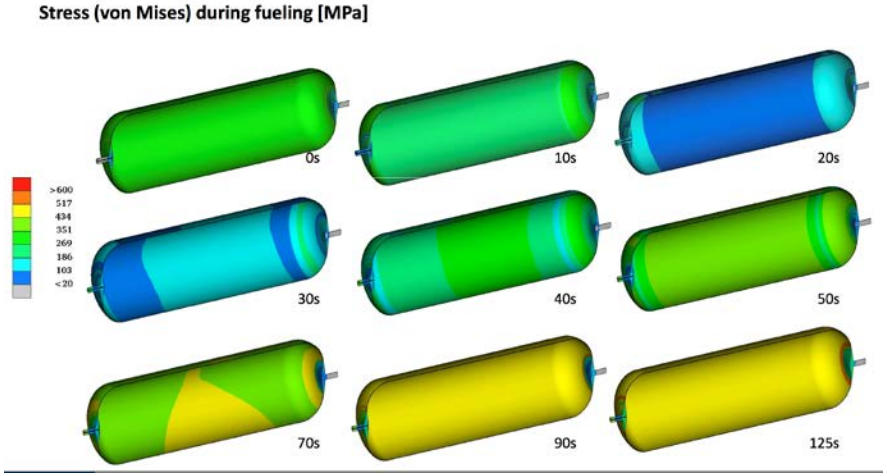
		Epoxy	Vinyl Ester
	Test Type	Relative Burst	Relative Burst
No Impact	Burst	105%	111%
	Cycle A	100%	103%
	Cycle B	99%	95%
Impact test round 1	Burst	57%	55%
	Cycle A	67%	DNF
	Cycle B	58%	63%
Impact test round 2	Burst	70%	82%
	Cycle A	55%	74%
	Cycle B	62%	67%



ST101

Cryo-compressed H_2 storage [LLNL/BMW/Linde/Spencer]

- Approach: Develop a thin-lined, high fiber fraction composite pressure capable, cryogenic vessel
- Goal: Demonstrate 3 kWh/kg and 1.7 kWh/L system capacities at 700 bar
- Installed new test facility for vessel cryo-compress cycle testing
- **Fluid and structural computational modeling of wall stress during refueling performed**



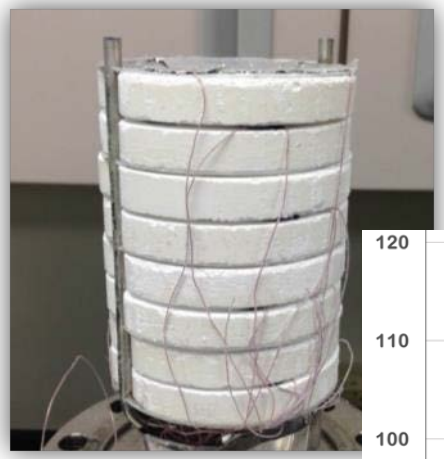
ST111

Cold and cryo-compressed H_2 storage for improved performance

Materials Based

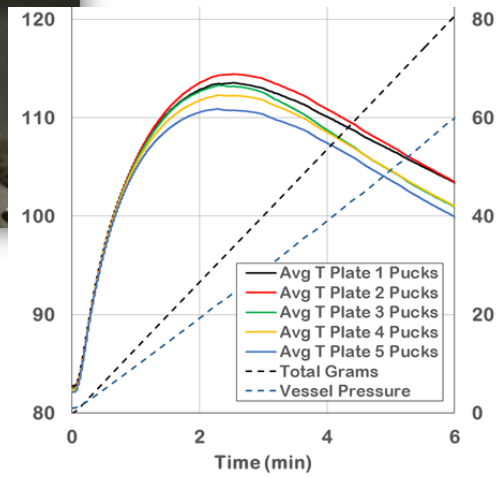
Accomplishments – H_2 Storage Engineering CoE

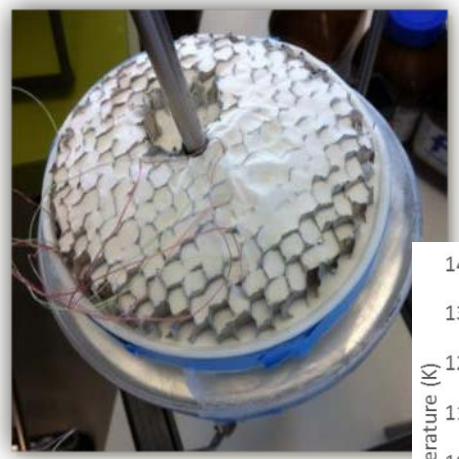
Evaluated two sorbent prototype systems for model validation:



MATI

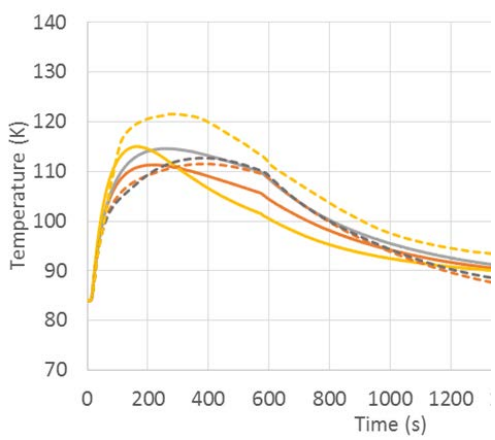
H_2Charging @ 150 SLPM





Hexcell

H_2Charging @ 100 SLPM, 80 Bar



Posted system models online for research community use: *http://HSECoE.org*

- MH acceptability envelope
- MH finite element model
- MH framework model
- Physical H_2 framework models
- Chemical hydrogen framework model
- Adsorption framework model
- Adsorption finite element model (coming)
- Tank volume/cost model

ST004 & ST008

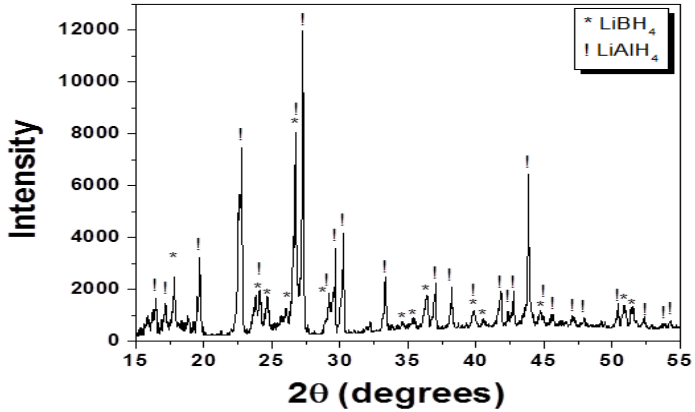
Online system models maintained and accessible to the research community

Accomplishments - Project Highlights

Low-cost methods for α-alane production [SRNL]

- Approach: Develop low-cost, efficient processes for alane synthesis
- Focused on improving electrochemical process for efficient α-alane production, coupled with
- Improving the recrystallization process of high-capacity α-alane
- **Achieved >99% recovery of electrolyte and additive materials**

Reagent recovery after α-alane recrystallization

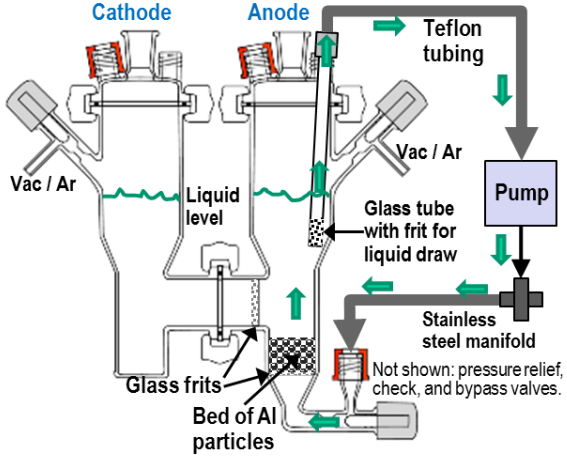


ST063

Low-cost methods for α-alane production [Ardica/SRI]

- Approach: Develop fluidized electrochemical process for low-cost commerical α-alane production
- Goal: Reduce alane production costs to less than $10/kg
- **Demonstrated successful isolation of an alane adduct from highly conducting $NaAlH_4$/THF electrolyte**

Schematic of particle bed electrochemical cell



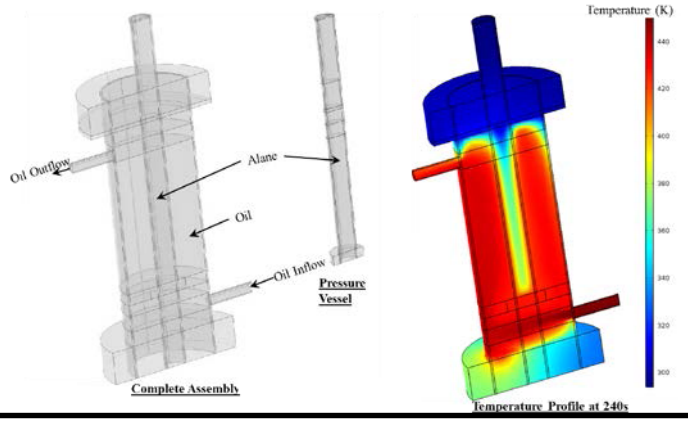
ST116

Low-cost α-alane production for commercial applications

Accomplishments - Project Highlights

Materials-based H_2 Storage for UUV Applications [SRNL/US Navy/Ardica]

- Objective: Screen H_2 storage systems to meet DoD targets and requirements for UUV applications.
- Goal: Develop complete system designs that meet Gen 1 and 2 requirements.
- Identified reversible (Gen 1) and non-reversible (Gen 2) materials that meet UUV targets
- Completed preliminary engineering analysis and proof-of-concept testing for an AlH_3 system
- **Preliminary analysis indicate 2-3 times energy storage compared to battery systems**

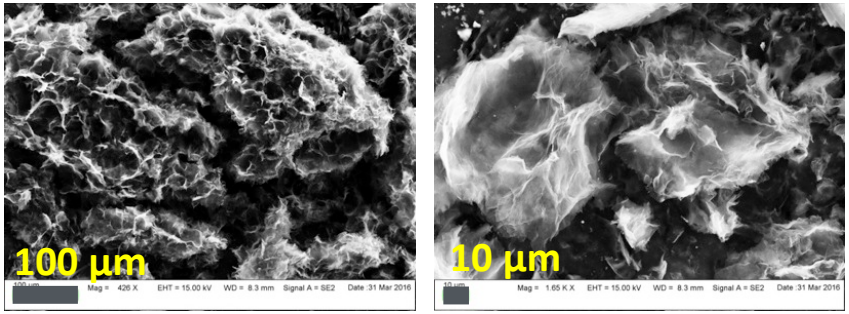


ST134

Design and Synthesis of Materials with High-Capacities for Hydrogen Physisorption [California Institute of Technology]

- Objective: Develop high performing H_2 adsorbents prepared from either graphene or exfoliated graphite.
- Goal: A hydrogen storage capacity of ≥ 11 wt.%, and near-constant isosteric heat of adsorption.
- Prepared activated graphene oxide material with 2336 m^2/g
- **Demonstrated metal functionalization of graphene via plasma deposition and chemical routes**

KOH activation of microwaved GO



ST120

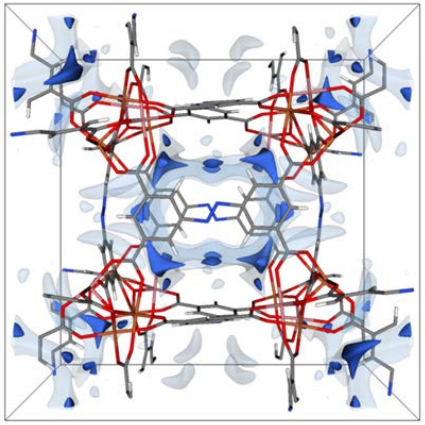
Leveraging HSECoE models and developing improved H_2 sorbents

Accomplishments - Project Highlights

High-Capacity & Low-Cost Hydrogen-Storage Sorbents for Automotive Applications [Texas A&M University]

- Objective: Develop metal-organic framework (MOF) sorbents with capacities exceeding the conventional storage limit per unit surface area
- Approach: Design MOF materials with high-valent metals to increase H_2 affinity relative to surface area to exceed the Chahine rule
- Performed detailed characterization, including activation and densification studies, of PCN-250
- **Measured 1.5x Chahine rule prediction for excess H_2 adsorption**

Potential energy contours for H_2 absorbed in PCN-250.

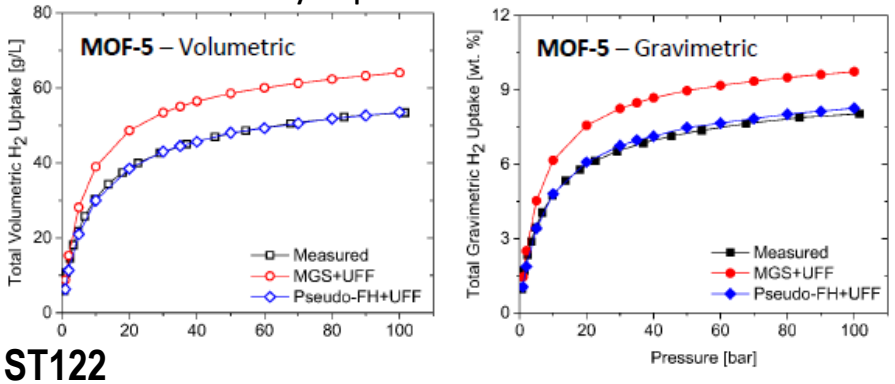


ST121

Hydrogen Adsorbents with High Volumetric Density: New Materials and System Projections [University of Michigan]

- Objective: Develop high volumetric adsorbents that also have high gravimetric capacities
- Approach: Investigate "best-in-class" sorbents identified through screening of reported structures in the Cambridge Structure Database
- Computationally screened over 2000 MOFs for adsorption capacity – identifying several promising candidates
- **IRMOF-20 synthesized and shown to have higher usable capacity than MOF-5**

Pseudo-FH force field appears to more accurately reproduce measurements



ST122

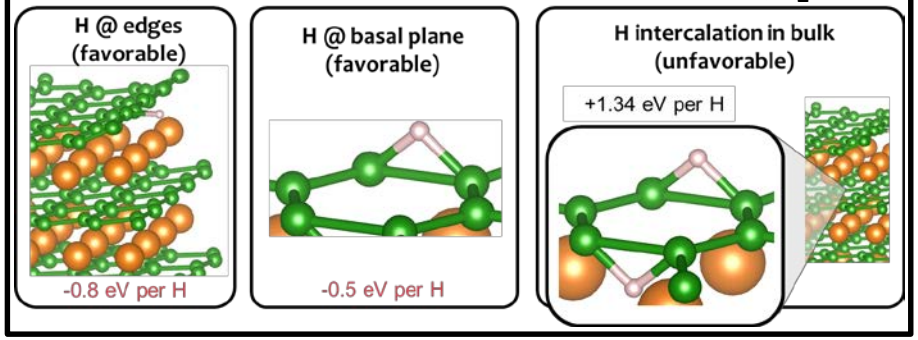
New MOF development targeting high volumetric capacities

Accomplishments - Project Highlights

Improved performance for $Mg(BH_4)_2$ [LLNL/SNL]

- Approach: Combined computational and empirical effort to identify ways to improve performance
- Goal: Develop flexible, validated, multi-scale model and use to develop practical material that satisfies DOE 2020 targets.
- Computed energetics of hydrogen in MgB_2
- **Experimental evidence supports proposed mechanism of selective hydrogenation of B atoms concentrated at interfaces in MgB_2, forming BH_4-like species**

Thermodynamic computations suggest hydrogen migrates to surfaces and interfaces of MgB_2

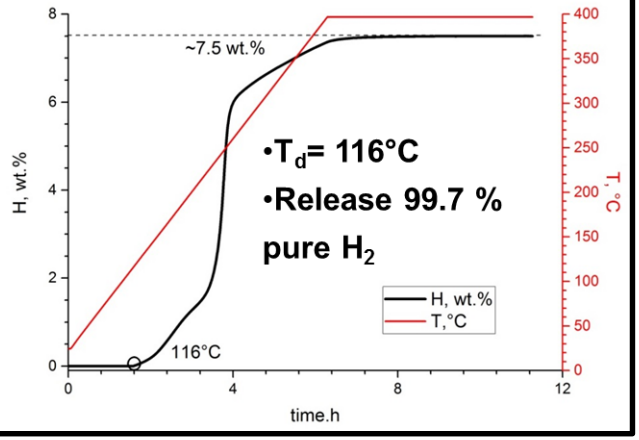


ST118

High-capacity Hydrogen-Storage Systems via Mechanochemistry [Ames Laboratory]

- Objective: Develop low-cost, reversible, high-performance H_2 storage materials
- Approach: Computational modeling to guide mechanochemical processing synthetic methods to produce hypersalts of silicon borohydrides
- Computational screening identified several metastable candidates to investigate
- **Investigated several novel systems with potential of over 17 wt.% theoretical H_2 capacity**

Desorption isotherm for "$LiSi(BH_4)_5$"



ST119

Boron-based, high-capacity H_2 storage materials

New Effort: HyMARC

Hydrogen Materials – Advanced Research Consortium

Individual projects

- **Applied material development**
  - Novel material concepts
  - High-risk, high-reward
- **Concept feasibility demonstration**
- **Advanced development of viable concepts**

Core National Laboratory Team

- **Material development tools**
  - Foundational R&D
  - Computational modeling development
  - Synthetic/characterization protocol development
- **Guidance to FOA projects**
- **Database development**

Characterization and Validation Team

- **Characterization Resources**
  - Validation of Performance
  - Validation of "Theories"
- **"User-facility" for FOA projects/HyMARC**
- **Characterization Method Development**

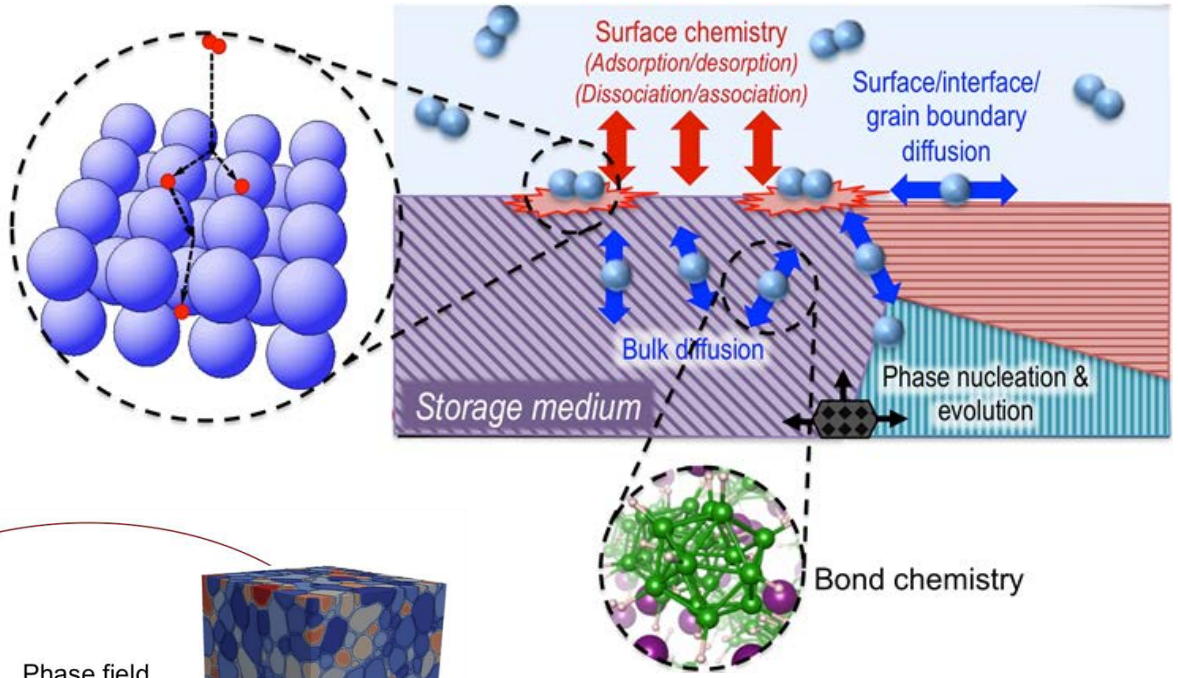


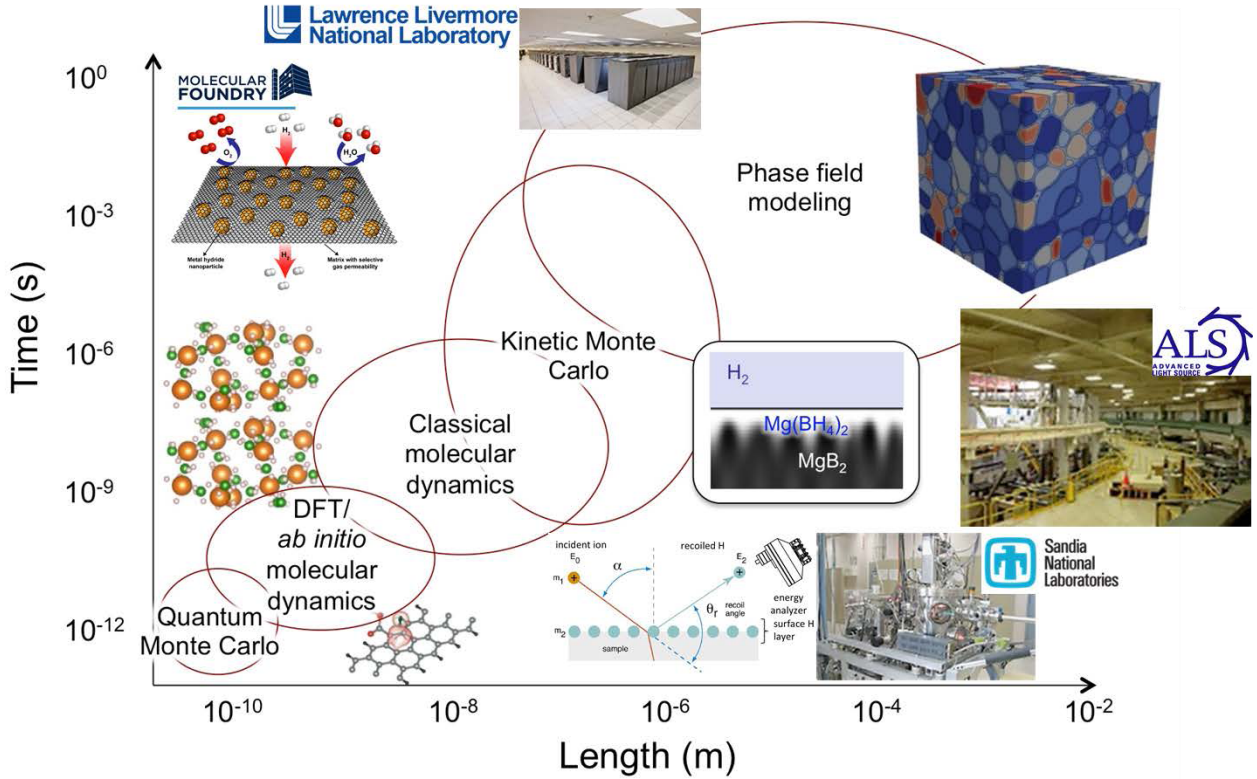
Part of the Energy Materials Network
U.S. Department of Energy

New Effort: HyMARC
The Core National Laboratory Team (SNL/LLNL/LBNL)

Address large gaps in the foundational science of hydrogen storage materials:

- Reaction thermodynamics
- Solid-state diffusion
- Surface chemistry
- Phase nucleation and microstructure
- Catalysis and additive behavior





Development of tools to accelerate development of hydrogen storage materials:

- Multi-scale, multi-physics computational materials design tools
- Advance materials characterization tools
- Synthetic protocols
- Database development

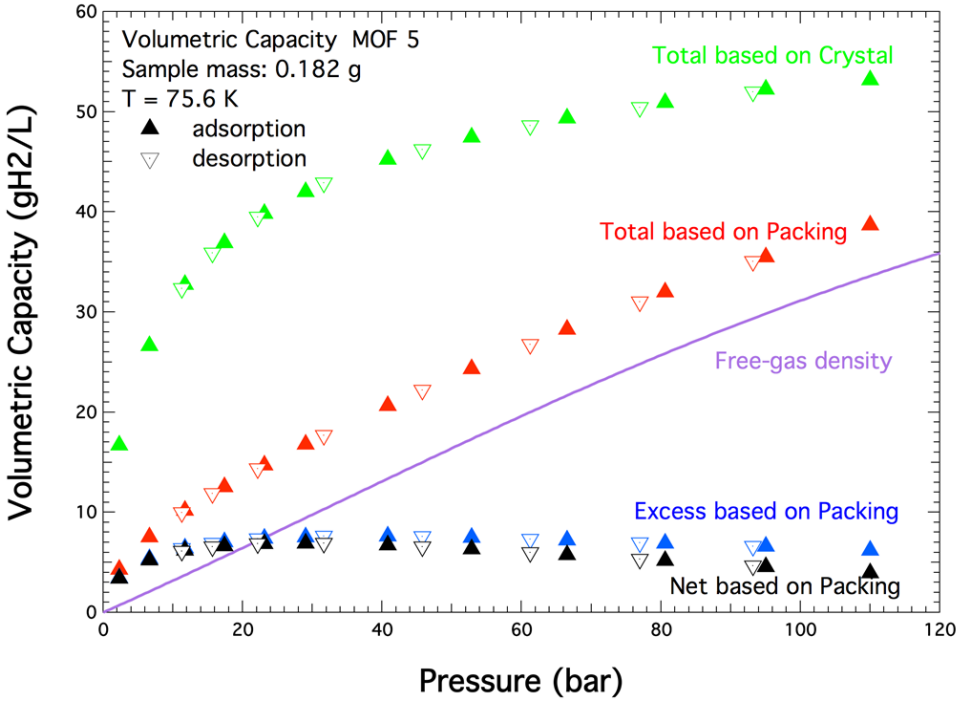
ST127; ST128; ST129; ST130

New Effort: The Hydrogen Storage Characterization and Validation Research Team (NREL/PNNL/LBNL/NIST)

Previously supported core characterization and validation capabilities combined into a coordinated effort:

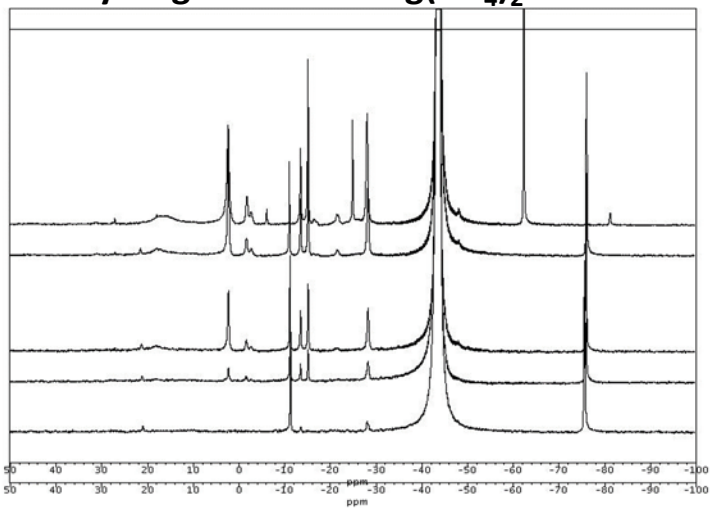
- To *Develop* and *Enhance* Core Characterization Techniques and Capabilities
- To *Validate* claims, concepts, and theories of hydrogen storage materials

Normalization of reporting of capacity volumetric data



ST014; ST131; ST132; ST133; ST135

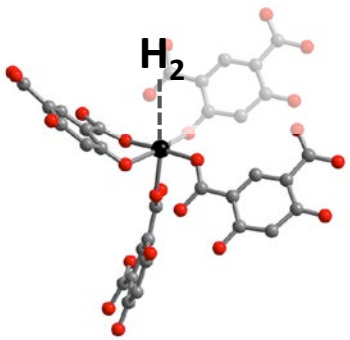
***In-situ* solid-state MAS ^{11}B NMR of the dehydrogenation of $Mg(BH_4)_2$ at 200 °C**



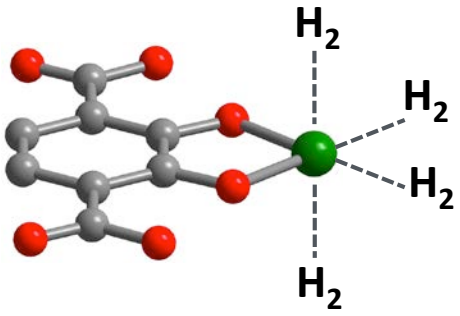
Suite of characterization capabilities available include:

- Variable temperature (cryogenic to high) H_2 adsorption measurements
- Variable temperature thermal conductivity
- Extensive NMR (liquid and solid-state)
- Microscopy
- Reaction calorimetry
- IR spectroscopy (DRIFTS)
- Various neutron methods:
  - Diffraction
  - Inelastic neutron scattering
  - Plus others

Major Achievement: *First example of multiple H_2 molecules adsorbed at a single metal center*

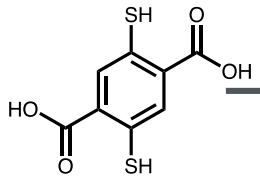


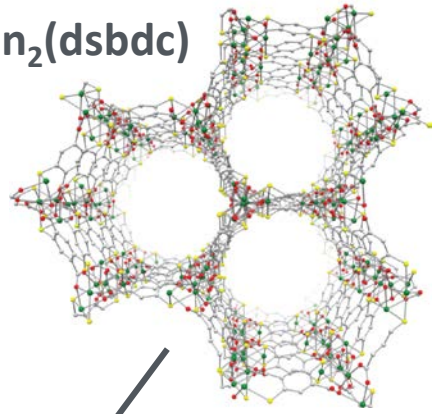
Traditional Materials:
1 H_2 per metal cation



Target Materials:
4 or more H_2 per metal cation??

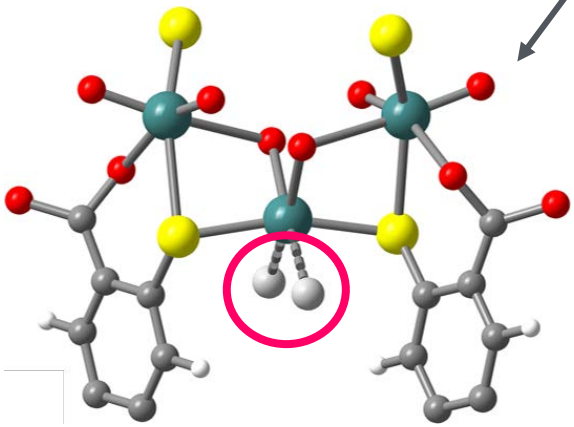
Mn^{2+} +





After desolvation the structure contains 4-coordinate Mn^{2+} atoms, which can adsorb 2 H_2 molecules

+ H_2



- Can we synthesize materials with under-coordinated metal sites?
- Materials with > 1 H_2 molecule adsorbed per site could display substantially increased volumetric capacities
- Mn_2(dsbdc) synthesized by **Jeff Long (UC-Berkeley/LBNL)**; neutron diffraction by **Craig Brown (NIST)**
- Meets FY16 GNG for NREL-led characterization team

First example of multiple H_2 molecules adsorbed at a single metal site

Runčevski, T.; Kapelewski, M. T.; Torres-Gavosto, R. M.; Tarver, J. D.; Brown, C. M.; Long, J. R. *Chem. Commun.*, submitted.

ST133; ST135

Demonstrates a synthetic path to materials with higher densities of adsorbed H_2

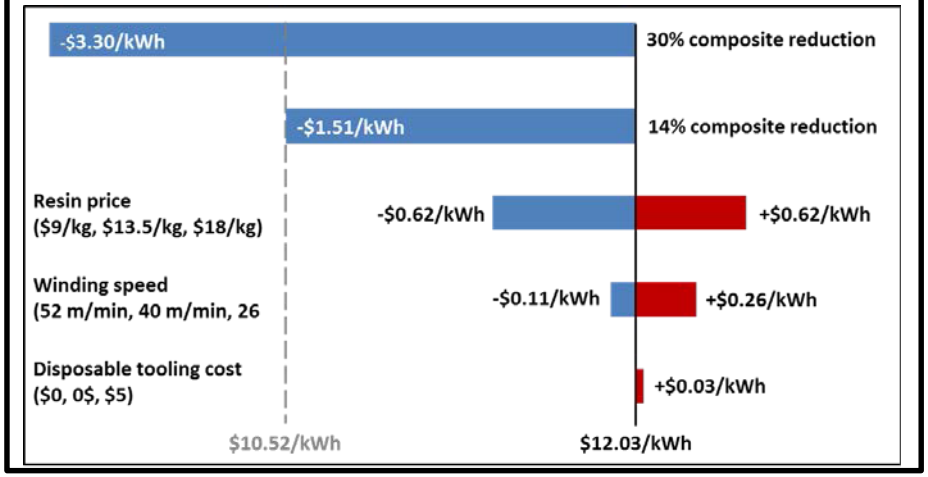
Analysis

Accomplishments- Highlights

Hydrogen Storage Cost Analysis [SA/ANL/NREL]

- Approach- Conduct "Design For Manufacture and Assembly" analyses of H_2 storage technologies
- Goal - To identify key R&D areas for Program to focus on to reduce system costs
- Performed trade-off analyses on COPV manufacturing processes
- **Completed preliminary analysis for the Materia project, indicating potential cost reduction**

Preliminary analysis for the Materia project

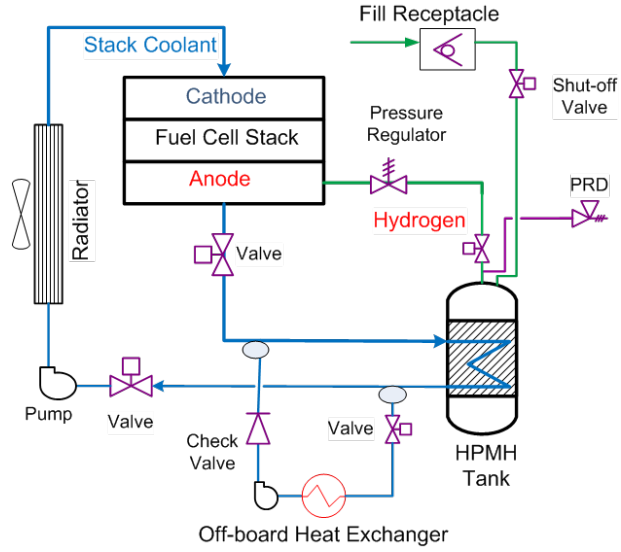


ST100

H_2 Storage System Performance Analysis [ANL]

- Approach- Conduct compete system analyses of H_2 storage technologies
- Goal - To identify key R&D areas for Program to focus on to meet performance targets
- Analyzed publically available information on Toyota Mirai H_2 COPV design for comparison with DOE baseline system
- **Determined properties for MH/350-bar hybrid systems to match/exceed performance of 700-bar systems**

350-bar Hybrid Storage System Schematic



ST001

Techno-economic and performance analyses used to target key R&D areas

New Efforts

- FY16 Office-wide FOA Topics:
  - Techno-economic analysis of onboard H_2 storage systems (1 selection announced – *Strategic Analysis Inc. with ANL & PNNL*)
  - Advanced insulation concepts for sub-ambient onboard H_2 storage systems (1-2 awards expected)
  - H_2 Storage Materials Discovery – HyMARC (multiple awards expected)
- Request For Information – *Cost Reduction and Performance Improvements of Composite Overwrapped Pressure Vessel Systems for Compressed H_2 for Onboard Vehicle Applications* (DE-FOA-0001596 – accessable through EERE eXCHANGE)
  - Open until June 30th
  - Responses are to be submitted to H2storage@ee.doe.gov
- Workshop on COPV system cost reduction strategies
  - To be held fall 2016
  - Dates and location still to be determined

RFIs and workshops used to identify annual FOA topics

Collaborations

INTERNATIONAL ACTIVITIES

- IEA HIA Task 32 Hydrogen-based Energy Storage

DOE – EERE - FCTO
Hydrogen Storage Applied R&D

- Physical Storage
- Fiber Composites
- Materials-based Storage
- System Engineering
- Testing and Analysis

INDUSTRY

- U.S. DRIVE Tech teams:
  - H_2 Storage
  - H_2 Delivery
  - Codes & Standards
  - Fuel Cells
  - Fuel Pathways
  - Vehicle Systems

TECHNOLOGY VALIDATION

National Collaborations (inter- and intra-agency efforts)

DOE - EERE	DOE – Office of Science	DOE – ARPA-E	DOC - NIST	DOD
VTO; BETO; AMO (i.e. IACMI) ; SETO	BES; ASCR		• Neutron scattering • Measurements	DOD/DOE MOU

Applied R&D is coordinated among national and international organizations

Recent and Upcoming Activities

Low-cost Compressed H_2 Storage Systems:

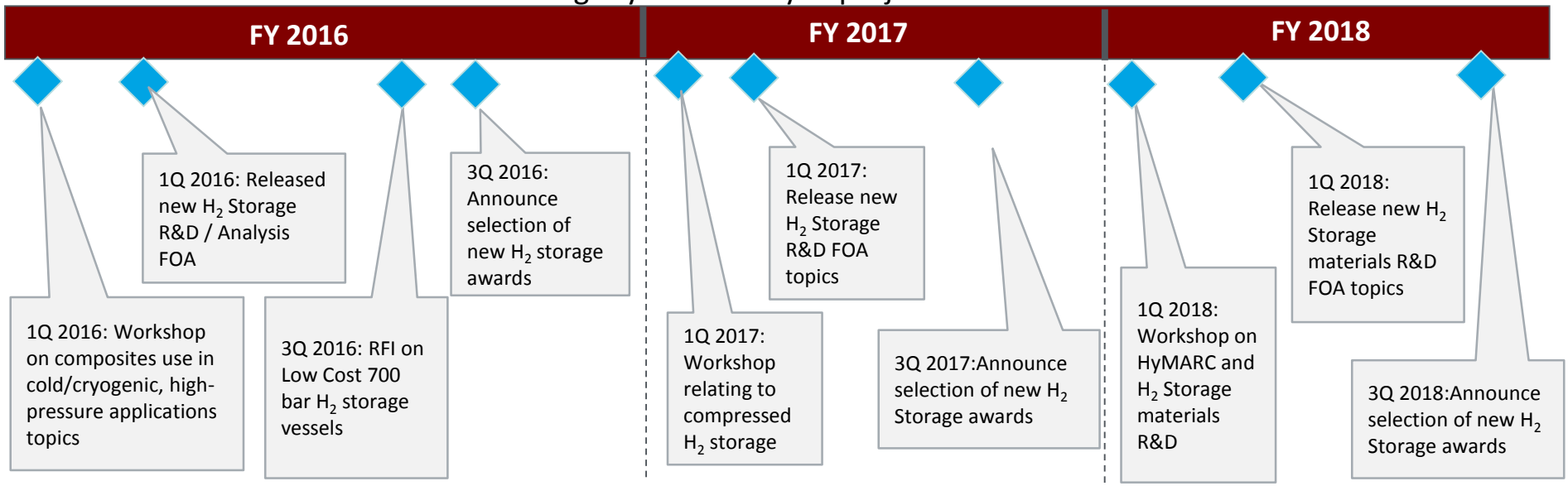
- Updated 700 bar compressed hydrogen system cost record to $15/kWh
- Announced selections for FY16 project(s) on advanced insulation for cold/cryogenic compressed H_2 storage
- Released RFI on strategies for improved performance, low-cost compressed hydrogen systems
- Engage with IACMI through AMO on compressed gas storage activities

Materials-Based Hydrogen Storage:

- Launched a revamped, coordinated hydrogen storage materials development effort:
  - HyMARC consortium (led by SNL)
  - Hydrogen Storage Characterization and Validation Research Team (led by NREL)
- HSECoE completed construction, testing and evaluation of two sorbent system prototypes and posted systems models for use by R&D community
- Announce selections FY16 projects to support HyMARC effort

Analysis

- Announced selection for FY16 H2 storage systems analysis project



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http://energy.gov/eere/fuelcells/fuel-cell-technologies-office