U.S. DEPARTMENT OF
ENERGY

Office of
ENERGY EFFICIENCY &
RENEWABLE ENERGY

H_2 Fuel R&D Overview

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2018 Annual Merit Review

June 13, 2018


H_2 Fuel R&D Addresses Program Priorities

Developing & enabling **transformational technologies** to sustainably produce & efficiently utilize large quantities of **affordable H_2** from diverse **domestic resources**

H2@Scale[SM]
U.S. Department of Energy

- ***Energy storage, energy security, grid resiliency, domestic employment, and energy innovation***

Leveraging **Consortium Model** to accelerate critical early-stage applied materials R&D for **hydrogen production**, **storage and distribution**

HydroGEN Advanced Water Splitting Materials

HyMARC Hydrogen Materials Advanced Research Consortium

HMat Hydrogen Materials Consortium

- ***H2@Scale depends on a future portfolio of large-scale, low-cost, sustainable H_2O splitting***
- ***Breakthrough H_2 storage materials are key to large-scale H_2 energy & future on-board storage***
- ***Foundational R&D to develop tools that predict and enhance materials compatibility, durability, and performance***

H_2 Fuel R&D Goals and Objectives

FCTO Early-Stage R&D Areas

Fuel Cells

- PGM- free catalysts
- Durable MEAs
- Electrode performance

PGM = Platinum group metals
MEA = Membrane Electrode Assembly

Hydrogen

- Production pathways
- Delivery components
- Advanced materials for storage

H_2 Production

- Enable **H_2 production at < $2/kg** utilizing diverse, domestic feedstocks

H_2 Delivery

- Reduce the cost of **delivery and dispensing to $5/kg by 2025 and ultimately $2/kg**

H_2 Storage

- Enable **$8/kWh for on-board H_2 storage cost**

Developing diverse affordable options for widespread H_2 adoption

H_2 Production & Delivery Cost Status and Targets

Targets

Early Market Target

$7/kg

$4/kg

Ultimate Target

Cost Status

(untaxed)

Low-Volume
early markets using NG

$16/kg to $13/kg

High-Volume*

$10/kg to $5/kg

*high-volume projections assume economies of scale

LOW-VOLUME

- **Early market status based on low-cost H_2 from NG (<$2/kg) plus delivery & dispensing**
- **R&D innovations are essential to reduce H_2 delivery & dispensing costs**

HIGH-VOLUME

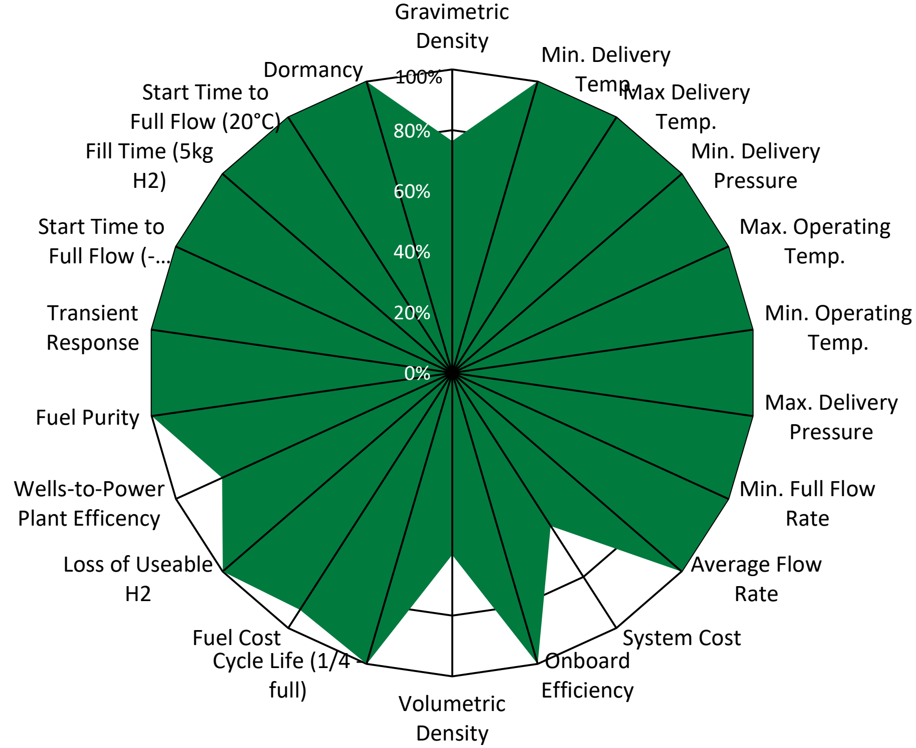
- **Projected status based on large-scale deployments of a portfolio of H_2 production, delivery & dispensing options**
- **R&D of diverse, sustainable hydrogen production pathways remains vital**

The full set of H_2 P&D targets can be found on the Program's website:
https://www.energy.gov/eere/fuelcells/downloads/fuel-cell-technologies-office-multi-year-research-development-and-22

H_2 Storage R&D Targets and Status

Storage Targets	Gravimetric kWh/kg ($kg\ H_2$/kg system)	Volumetric kWh/L ($kg\ H_2$/L system)	Costs [1] $/kWh ($/kg H_2)
2020	1.5 (0.045)	1.0 (0.030)	$10 ($333)
2025	1.8 (0.055)	1.3 (0.040)	$9 ($300)
Ultimate	2.2 (0.065)	1.7 (0.050)	$8 ($266)
Current Status [2]			
700 bar compressed (5.6 kg H_2, Type IV, Single Tank)	1.4 (0.042)	0.8 (0.024)	$15 ($500)

700 Bar Compressed Status[2] vs. 2025 Targets



[1] Projected at 500,000 units/year

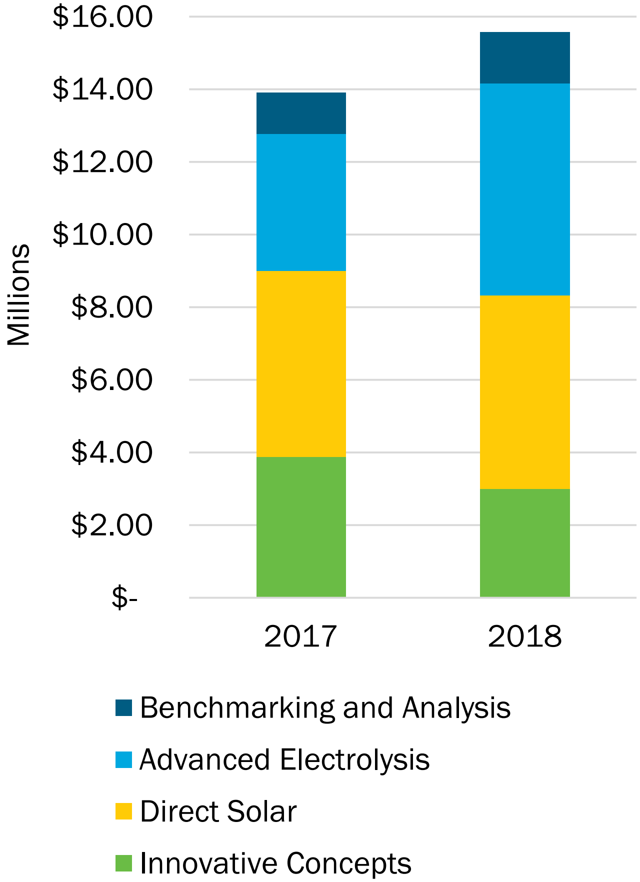
[2] FCTO Data Record #15013, 11/25/2015: https://www.hydrogen.energy.gov/pdfs/15013_onboard_storage_performance_cost.pdf

The full set of H_2 storage targets can be found on the Program's website:
https://energy.gov/eere/fuelcells/downloads/doe-targets-onboard-hydrogen-storage-systems-light-duty-vehicles

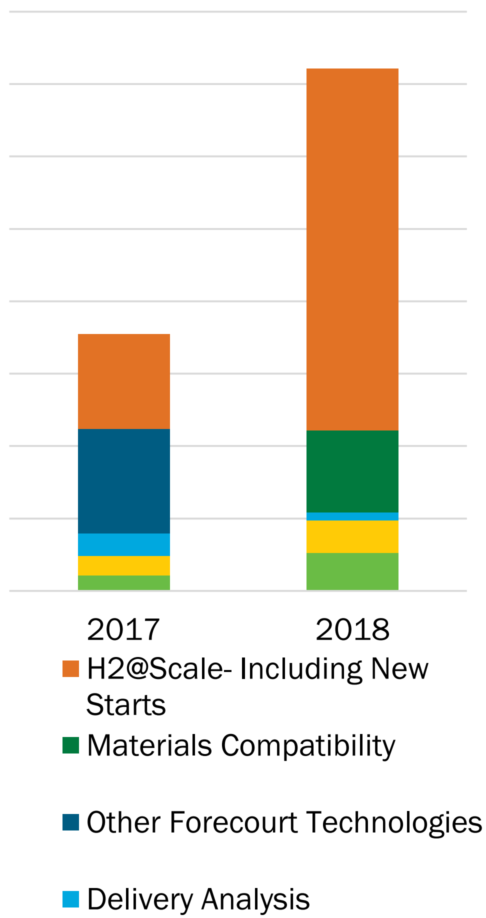
H_2 Fuel R&D Funding

Appropriations: FY17: $41M; FY18: $54M

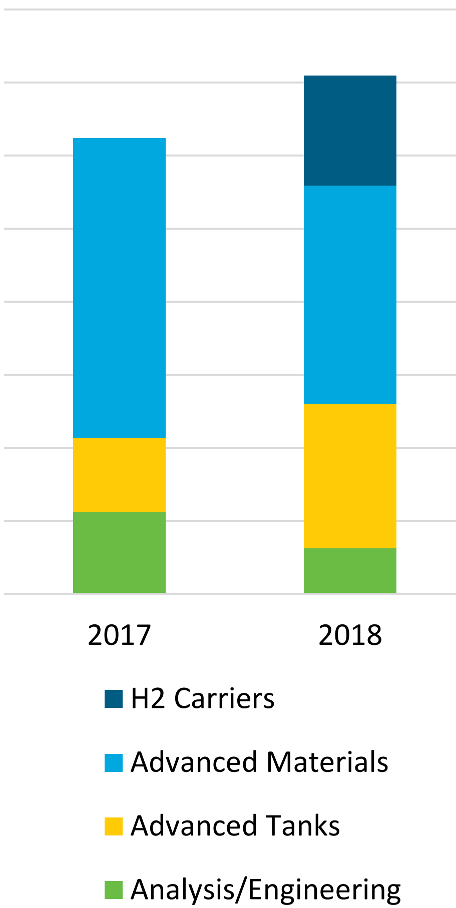
Production



Delivery



Storage



Research priorities guided by H2@Scale are reflected in annual adjustments

Effective Teamwork: H_2 Interface Task Force

Diverse Production Options

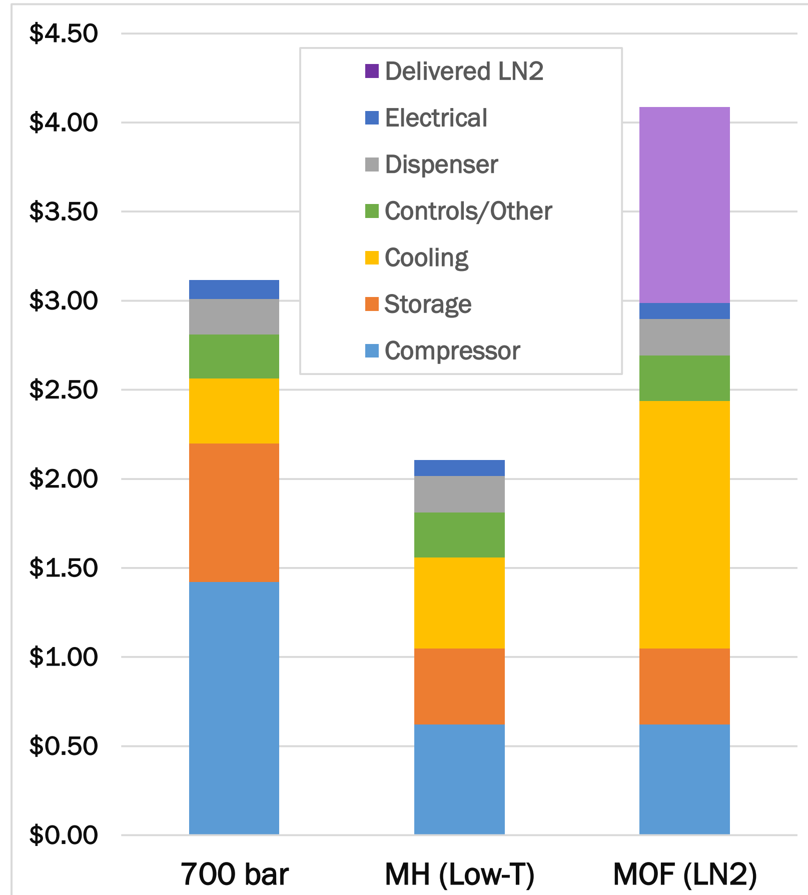
Onboard Storage Technology

Delivery Infrastructure Options

	700 bar	Cold-compressed	Cryo-compressed	Cryo-sorbent	Metal Hydride
Liquid H_2	★	★	★	★	★
Low P (<200 bar)	★			☆	★
High P (>200 bar)	★			☆	★
Pipeline	★			☆	★
Forecourt Implications	Pre-cooling to -40 °C	Refrigeration to 150 K	Supercritical H_2 (<150K)	Cooling to ~80 K	Heat rejection

Delivery & Dispensing Cost [2016$/kg H_2]

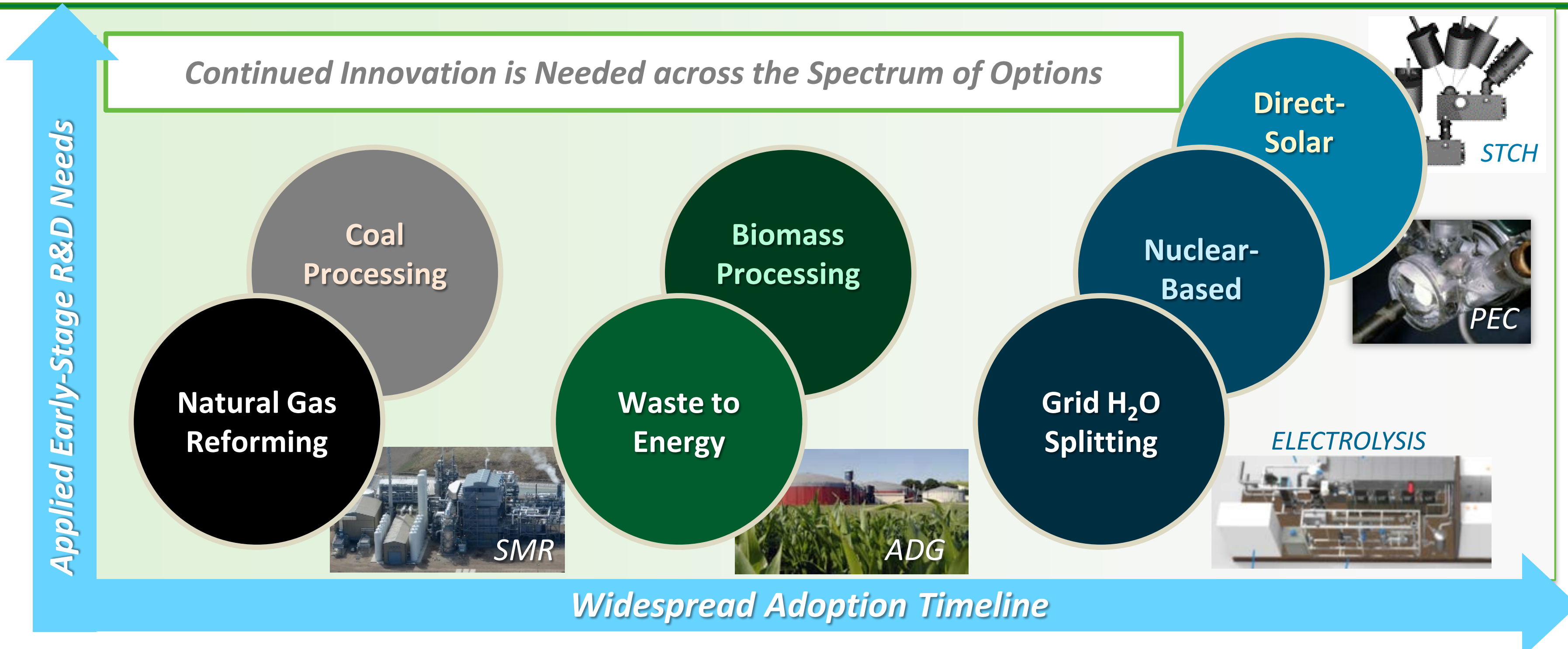
Preliminary **SA170**



H_2IT looks at issues associated with coupling refueling infrastructure options with onboard storage technologies

Hydrogen Production

H_2 Production from Diverse Domestic Resources



FOSSIL RESOURCES

- Low-cost, large scale H_2 production with CCUS options
- New options offer scalability and byproduct benefits (e.g. CHHP)

WASTE/BIOMASS

- Options include innovative biogas reforming & fermentation of waste streams
- Byproduct benefits include clean water, electricity & chemicals

WATER SPLITTING

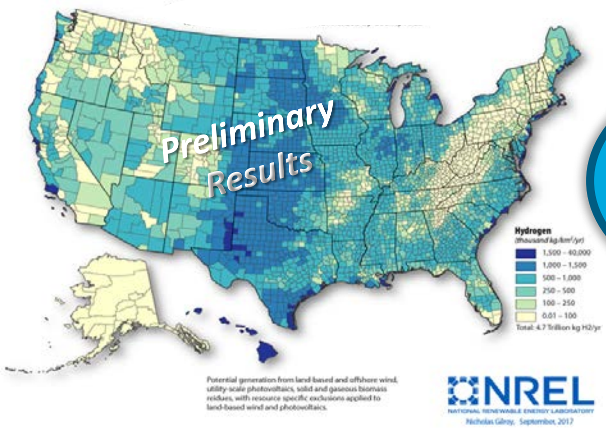
- Grid electrolysis is proven process being improved with innovation
- Emerging nuclear/solar options offer long-term sustainable H_2

A broad portfolio of near- to longer-term H_2 production technology options is being addressed through early-stage R&D

Production R&D Strategies and Focus Areas

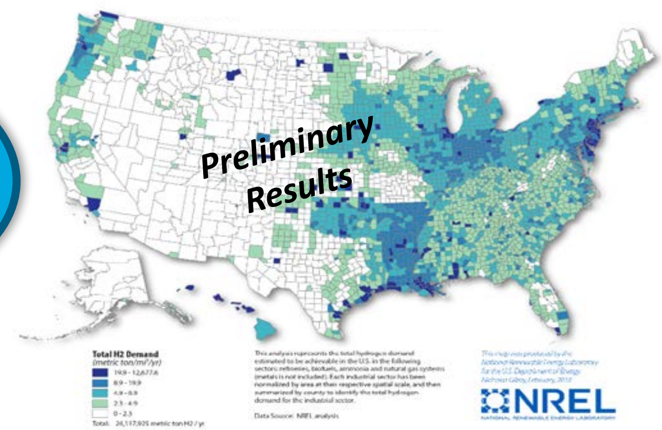
Challenge	Strategies	R&D Focus	Key Areas
Sustainable Low-Cost H_2 Production	***Foundational and Applied Research***	***Research Guided by Techno-economics***	***Enable H_2 production from diverse domestic resources***
• **Materials efficiency** • **Feedstock use** • **Capital costs**	• **Foundational R&D to enable broad H_2 production options including renewable, fossil and nuclear opportunities**	• **Early-stage materials R&D addressing key challenges in energy conversion, catalysis, separations, hydrogen compatibility, etc.**	• **Advanced water-splitting** • **Waste & bio-conversion** • **Nuclear/hybrid approaches**

H_2 Supply Potential from Diverse Domestic Resources



H_2 Production R&D Enables New Supply/Demand Opportunities

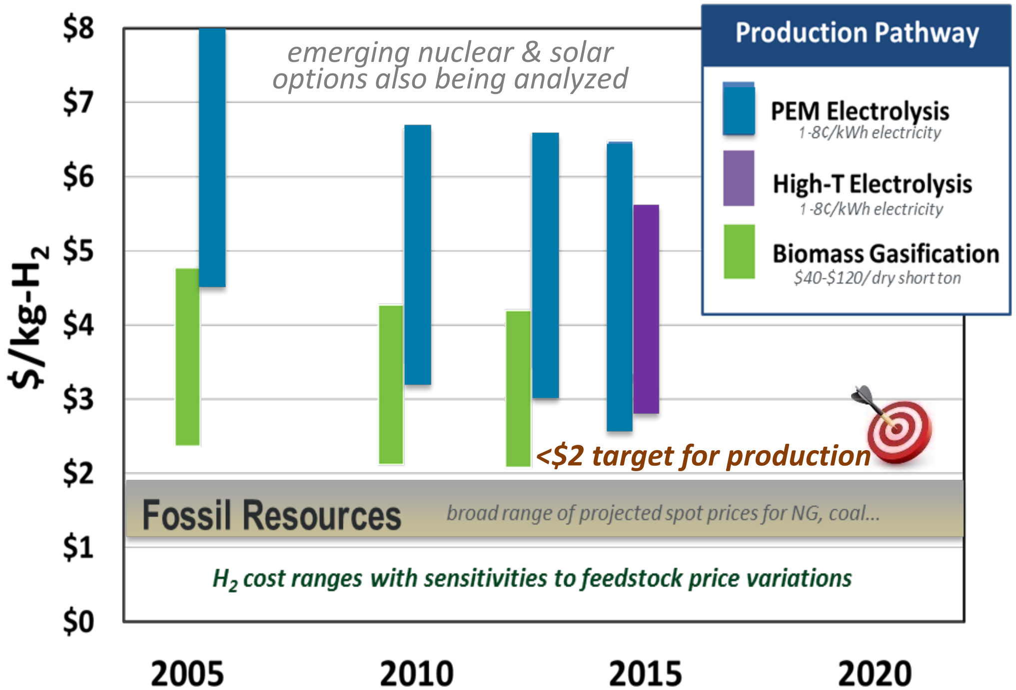
Potential H_2 Demand Growth by U.S. Region



Leveraging resources to optimize research impact on diverse H_2 production options, enabling long-term US energy independence with export opportunities & regional job creation

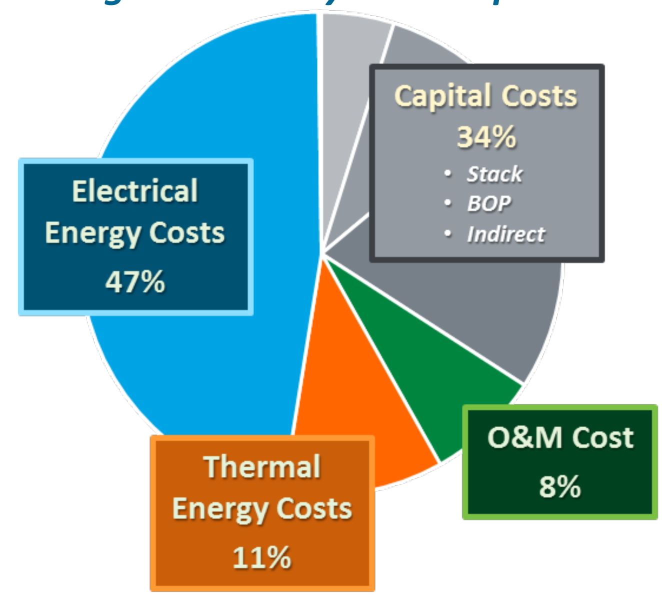
R&D Impact on H_2 Production Costs

Enhancing affordability of diverse options



Techno-economic levers for reducing costs

High-T electrolysis example



Early-Stage Applied R&D:

- *Innovative Reactor Concepts*
- *Novel Devices & Components*
- *Materials Compatibility*

Foundational Research:

- *Breakthrough Materials: catalysts, separators, thermal & optical materials…*

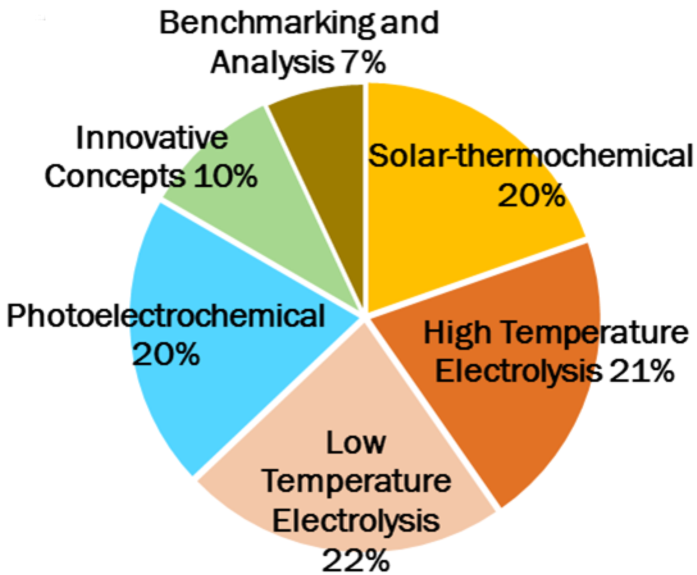
Innovative early-stage applied R&D is addressing the cost-competitiveness of H_2 production from diverse, sustainable domestic resources

Balanced R&D Portfolio Leveraging Diverse Resources

funding distribution in FOA, LAB, & SBIR/STTR projects

including % of portfolio funding by research topic area

H_2 Production



CURRENT EMPHASIS

- **Support R&D needs identified through the H2@Scale initiative:**
  - *Early-stage R&D on water-splitting technologies through the HydroGEN Consortium*
  - *Early-stage R&D exploring innovative production concepts from diverse national energy sources and feedstocks*
- **Continue leveraging cross-program, cross-office and cross-agency R&D opportunities and resources**

R&D Support Framework:

- FCTO FOA & Lab Calls
- H2@Scale Ecosystem
- DOE MOUs: NSF & NIST
- SBIR/STTR
- Crosscuts: EMN/Grid…
- NE, FE, SETO, BETO,WTO, GTO, WPTO

Recent High-Impact Collaborative Initiatives

- **Nuclear Energy**
  - *3 new H_2 production projects supporting nuclear-compatible production in high temperature electrolysis*

- **Fossil Energy / NETL**
  - *Supporting R&D work on NG decomposition to produce CO_2-free H_2 & higher value solid carbon products, including work with UCFER*

- **Basic Energy Sciences & SETO**
  - *Congressionally-directed effort to develop a solar fuels research initiative strategic plan*

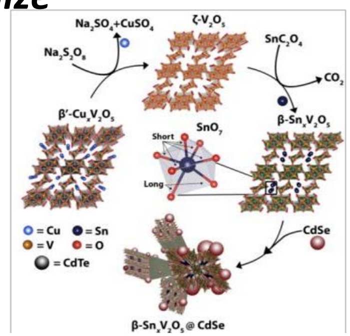
- **NSF-DMREF / HydroGEN EMN**
  - *Leveraging MGI methodologies integrating theory, experimentation & data to accelerate advanced water splitting materials discovery*

HydroGEN/NSF-DMREF Collaboration:
Four new projects selected for negotiations!

TEXAS A&M UNIVERSITY | BINGHAMTON UNIVERSITY, STATE UNIVERSITY OF NEW YORK | University at Buffalo

A Blueprint for Photocatalytic Water Splitting: Mapping multidimensional compositional space to simultaneously optimize thermodynamics & kinetics

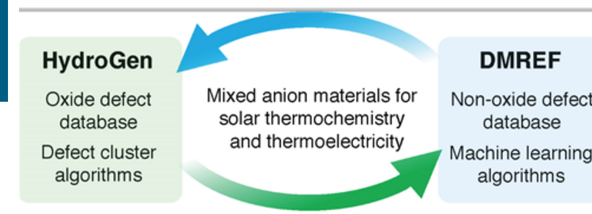
In-situ soft XAS/RIXS studies of identified nano-engineered photocatalysts



Colorado School of Mines | SLAC NATIONAL ACCELERATOR LABORATORY | ILLINOIS, UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

Advancing machine learning prediction algorithms for defects & dopability

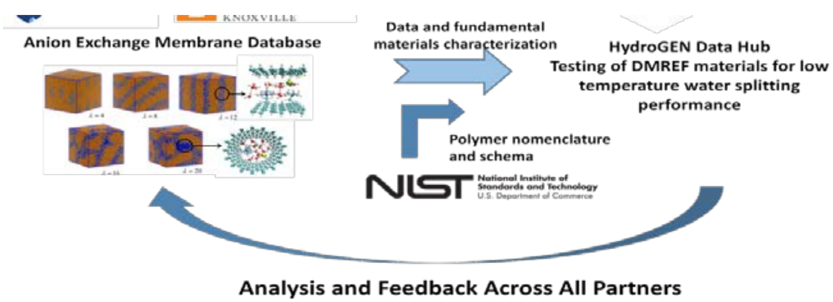
High Temperature Defects: Linking solar thermochemical and thermoelectric materials



Populating Data Hub with AEM results, accelerating the design of new AEMs for water splitting electrolyzers

Rensselaer | NYU | PennState | THE UNIVERSITY OF TENNESSEE KNOXVILLE

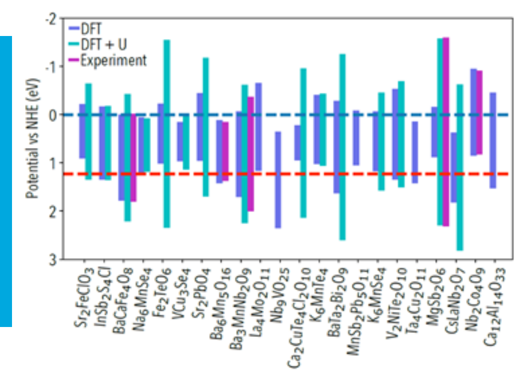
Membrane Databases: New schema and dissemination



PennState | Cornell University

Experimental validation of designed photocatalysts for solar water splitting

Integrated approach combining theory, computation, & experiment to discover promising water splitting photocatalyst materials

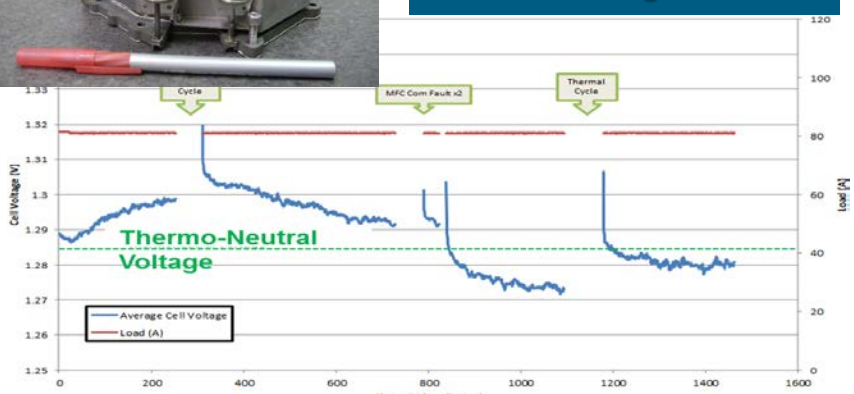


H_2 Production Project Accomplishments

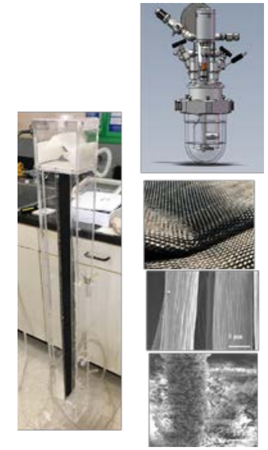
Winner of the $1 million H2 Refuel H-Prize, exports one of the world's first H_2 refueling appliances to Japan

TV041

45 cell stack exceeded 1000 hr operation at 97% LHV efficiency at 1 A/cm² (>3 kg H_2/day) with no discernible degradation

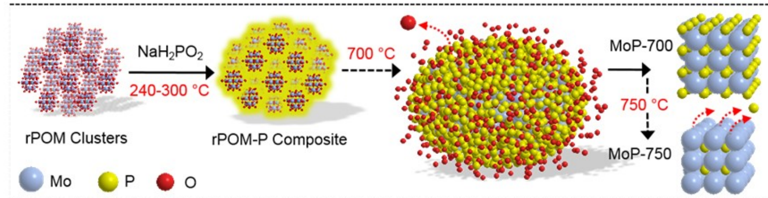


PD129



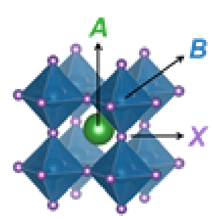
Demonstrated > 20 L/L/day H_2 produced using integrated Fermentation/MEC reactor

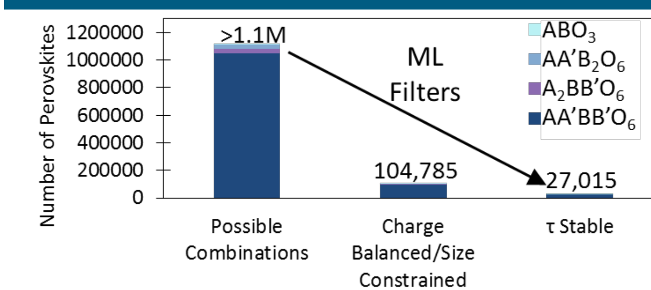
Patent application filed on novel MoP cathode catalyst with comparable performance to Pt.



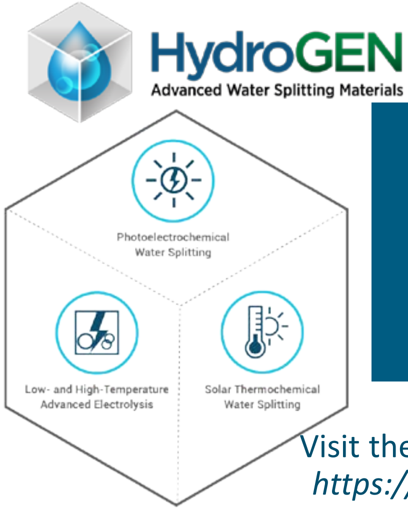
PD166

>1.1 M perovskites filtered using Machine Learning to 27,015, significantly reducing the # of computationally expensive DFT calculations





Pioneering Research in Water Splitting: HydroGEN

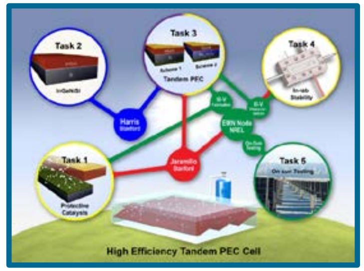


Fostering breakthroughs in catalysis, membranes, photoabsorbers, redox materials, & more!

Visit the HydroGEN website
https://www.h2awsm.org

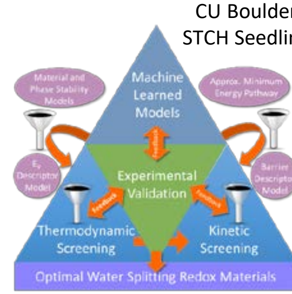
HydroGEN Seedling Projects

19 Seedling Projects Initiated
44 unique nodes utilized across core labs
> 100 samples exchanged



Stanford University PEC Seedling

CU Boulder STCH Seedling



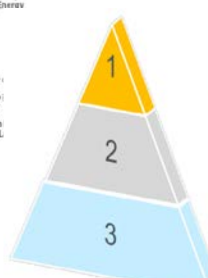
Streamlined Access

- **Non-Disclosure Agreement (NDA)** → Information Disclosure
- **Intellectual Property Management Plan (IPMP)** → IP Protection
- **Materials Transfer Agreement (MTA)** → Freedom to Operate
- **Cooperative Research and Development Agreement (CRADA)** → Collaboration (nearly complete)

National Innovation Ecosystem

> 80 unique, world-class capabilities/expertise

58 PEC	**39 HTE**
39 STCH	**46 LTE**
8 Hybrid Thermochemical	



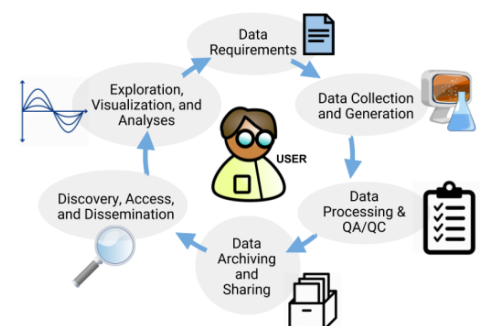
Category 1
Node is fully developed and has been used for research projects

Category 2
Node requires some development

Category 3
Node requires significant development

HydroGEN Data Hub: A Researcher Centric Approach

134 users & >240 files



- Secure project space for team members
- Metadata tools to support advanced search
- Link to other data repositories or databases
- Data plug ins for visualization

Energy Materials Network U.S. Department of Energy | NREL | Berkeley Lab | Sandia National Laboratories | INL Idaho National Laboratory | Lawrence Livermore National Laboratory | SRNL | U.S. Department of Energy Energy Efficiency & Renewable Energy

The HydroGEN Research Community

- HydroGEN Overviews: **6 oral presentations this afternoon** covering LTE, HTE, PEC, STCH, and Benchmarking & Protocols
- **Poster Session tonight** showcasing **18** new projects in AWS materials discovery & development

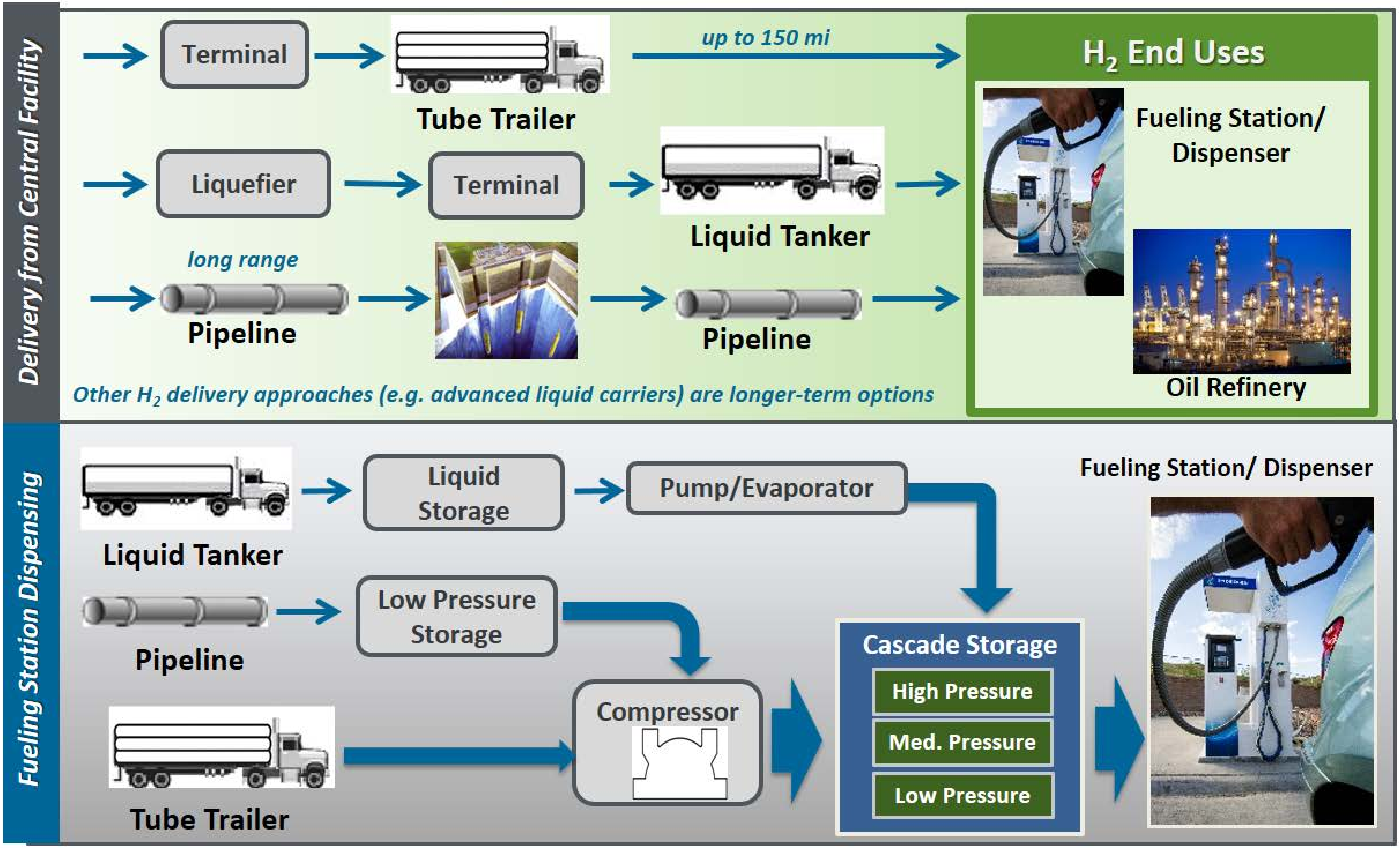
Rm: Lincoln 5
3:15-6:15 PM

Exhibit Halls B & C
6:30-8:00 PM

HydroGEN kicked off a collaborative nationwide R&D effort Nov. 2017

Hydrogen Delivery

Hydrogen Delivery Pathways

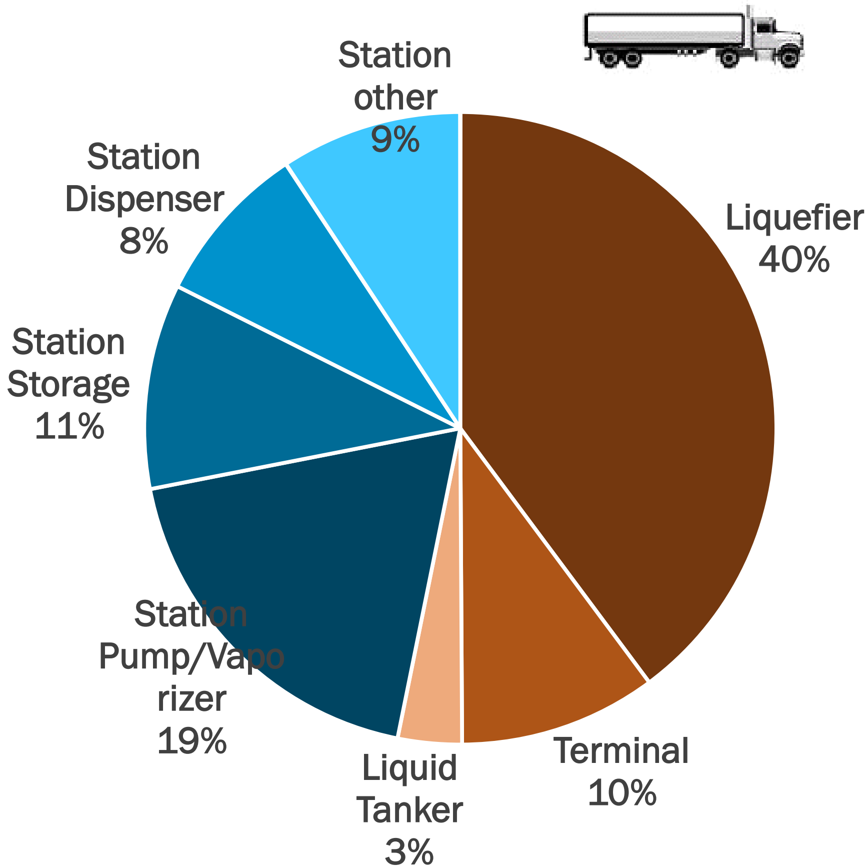


Continued R&D on affordable delivery & dispensing is key to enabling large-scale benefits of hydrogen

Hydrogen Delivery Challenges and Strategy

Projected Hydrogen Delivery Cost Breakdown

Example: Liquid Pathway Early Market



Key assumptions:
1,000 kg/day station, 1% market penetration,
low-volume manufacturing, 80% utilization in 5 years

Analysis Source: Hydrogen Delivery Scenario Analysis Model (HDSAM)

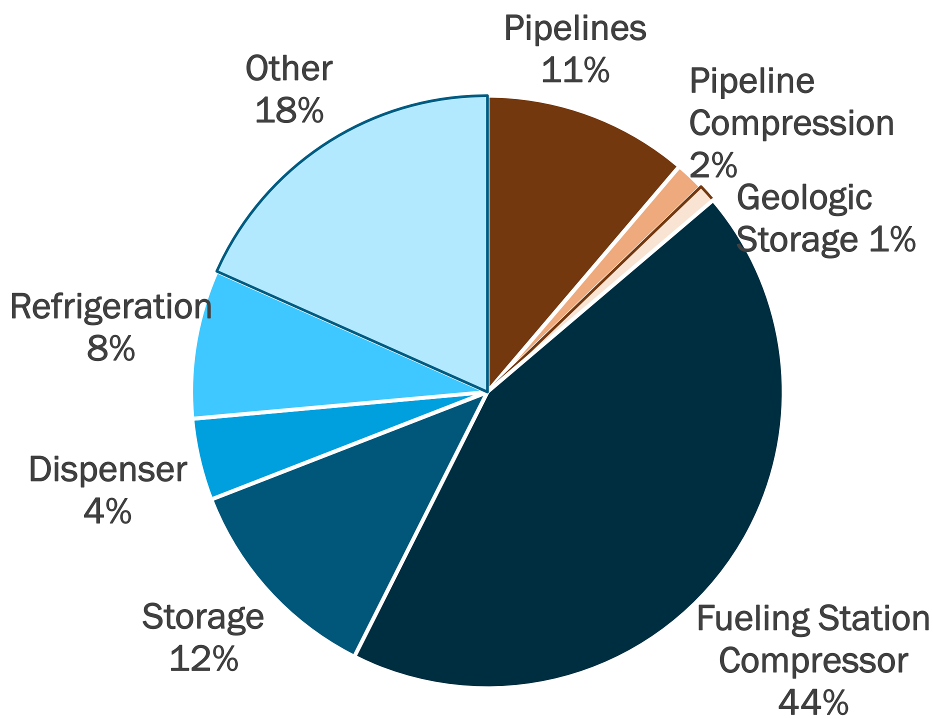
CURRENT R&D Focus Areas

- Non-mechanical approaches to **liquefaction** (e.g. magnetocaloric materials)
- Thermodynamic analysis of liquid hydrogen transfers and **boil-off mitigation** strategies.
- Wire-wrapped pressure vessels for **low-cost storage**
- **Novel hoses** for reliable, low-cost dispensing
- FY18: Reduction of **station footprint**, improvements in **component reliability**, mitigation of **liquid hydrogen boil-off**, and innovations in hydrogen **liquefaction**

Hydrogen Delivery Challenges and Strategy

Projected Hydrogen Delivery Cost Breakdown

Example: Pipeline Delivery, Mature Market



Key assumptions:
3,000 kg/day station, 70% market penetration, high-volume manufacturing

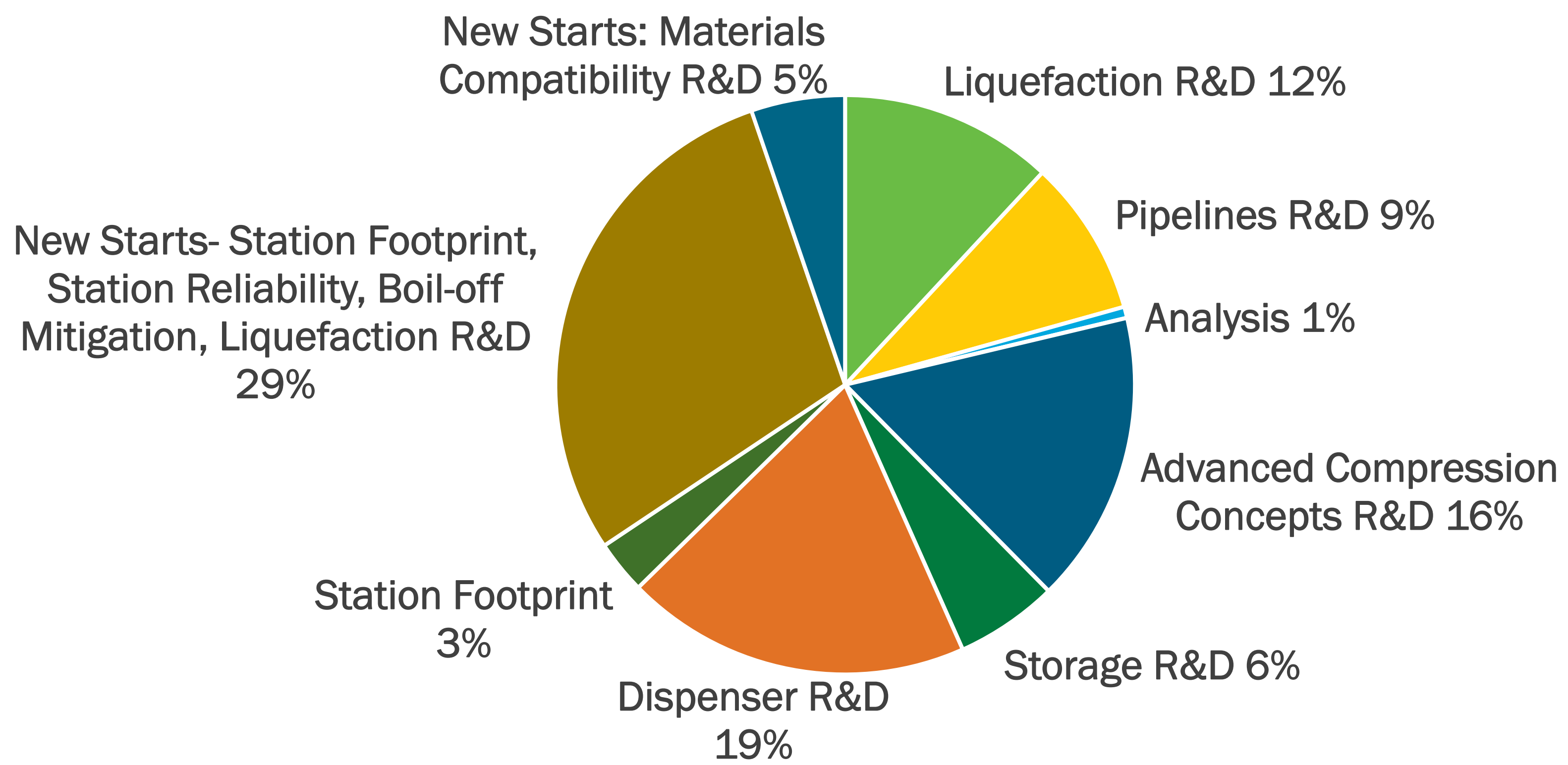
Analysis Source: Hydrogen Delivery Scenario Analysis Model (HDSAM)

FY18 R&D Focus Areas

- Use of modern, **high-strength steels** in hydrogen pipelines
- Computational modeling of **hydrogen effects in infrastructure** steels
- Novel concepts for **compression** (electrochemical, metal hydride) to improve reliability
- Innovative integrations of station **compression and storage** to reduce capital cost

Hydrogen Delivery Funding Distribution

Funding distribution in FOA, Lab, and SBIR/STTR Projects[1]



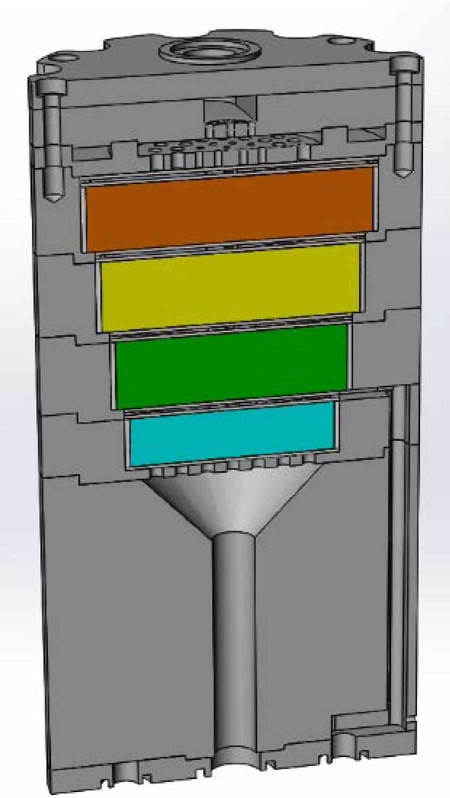
Collaborations

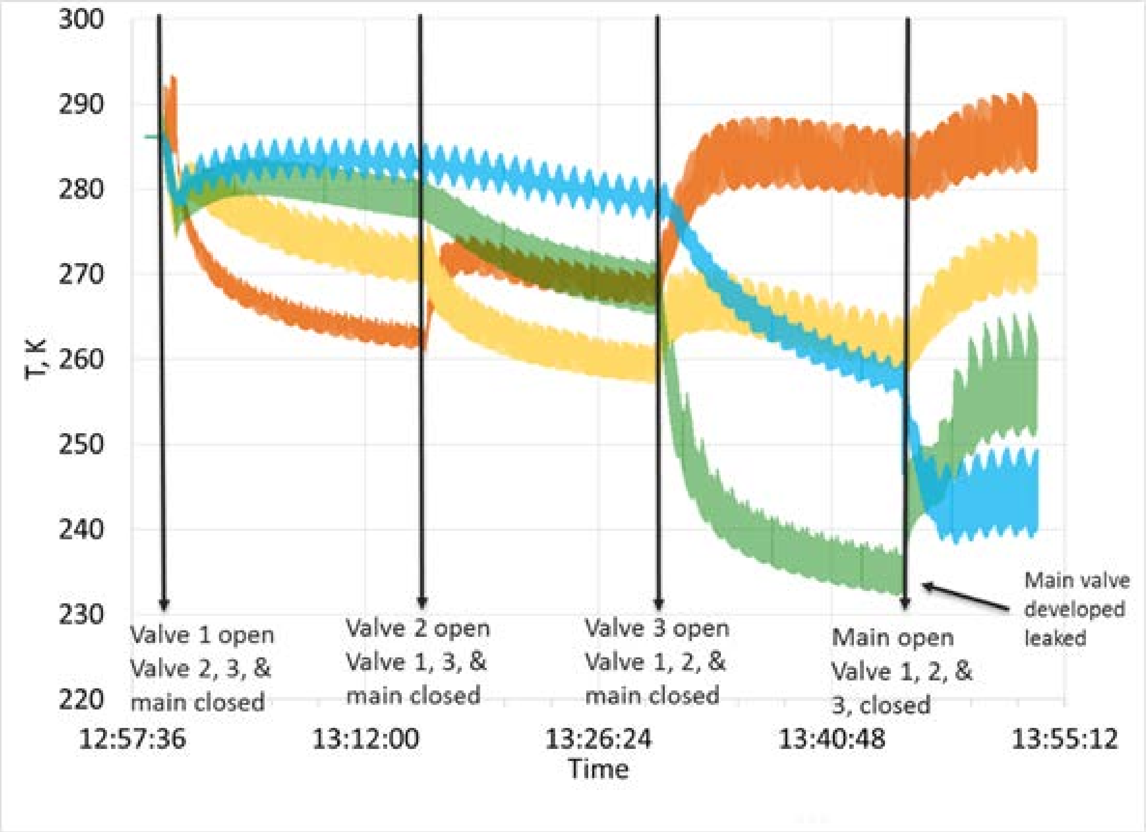
1. Distribution represents total project funding for any project ongoing in FY17

- DOE Office of Science (SBIR/STTR)
- Inter-agency (MOU)
- U.S. DRIVE
- IPHE
- H2@Scale

Hydrogen Liquefaction Technical Accomplishments

Exploratory R&D in magnetocaloric hydrogen liquefaction concepts with potential for 50% improved efficiency over conventional liquefaction

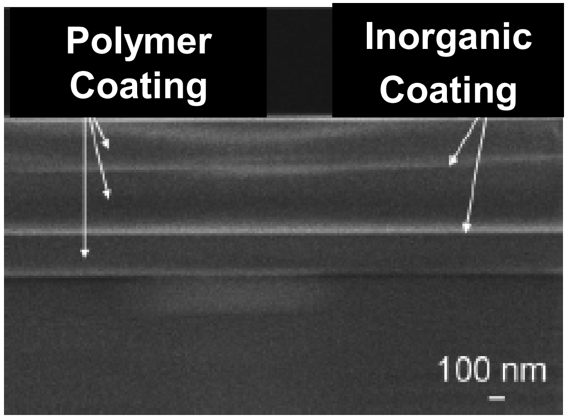




***Variable diversion flow valves control flow of heat transfer fluid to manage temperatures of magnetocaloric materials within regenerator** (PD131)*

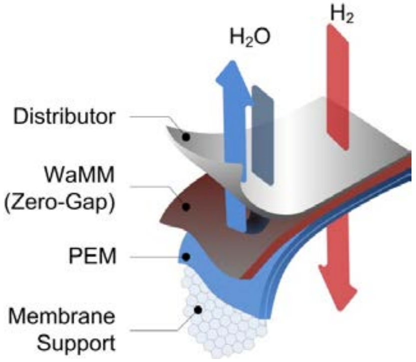
Pacific Northwest National Lab
Ames Laboratory
Emerald Energy Northwest, LLC

Hydrogen Compression Technical Accomplishments

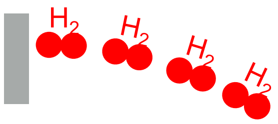


Innovative approach to coating compressor seals reduces erosion by 70%.

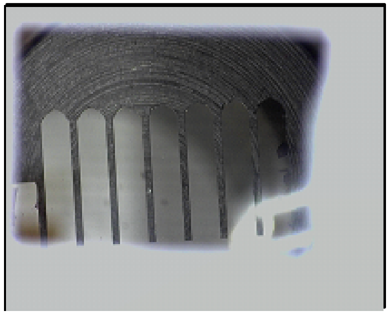
(GVD Corporation, Powertech, NREL, PD 150)



Reduced voltage required for 350-bar electrochemical compression by 50%.
(Giner, NREL, RPI, Gaia, PD136). ***2016 baseline***



Hydrogen absorption on metal hydrides deposited on cantilever beams



Use of machine learning and high-throughput experimentation to initiate computational model of metal hydrides

(Greenway Energy, NIST, SRNL, Univ. South Carolina, SBIR)

Future Direction: Hydrogen Materials Compatibility Consortium

HMat
Hydrogen Materials Consortium

Early-stage R&D on hydrogen effects on polymeric and steel materials in hydrogen technologies.

Collaboration across Delivery; Storage; Safety, Codes, and Standards

Materials compatibility influences reliability and cost of key technologies, such as:

Dispensing Hoses

Hydrogen Storage

Hydrogen Piping

Hydrogen Storage

H_2 Storage Early Stage R&D Approach

High-Pressure and Cryogenic

High Pressure (700 bar)

- Lower cost carbon fiber (CF)
- Improved composites
- Conformable designs
- Lower cost materials for balance-of-plant

Cold/Cryo-compressed (Low Temp.)

- System engineering
- Materials of construction
- Advanced insulation
- Improved dormancy

Advanced Materials

Solid-State Materials

Breakthrough materials to enable 2X the energy density compared to current systems:

- Foundation R&D carried out by lab team
- Innovative materials concepts carried out through individual projects
- Progress accelerated though lab interactions

HyMARC
Hydrogen Materials Advanced Research Consortium

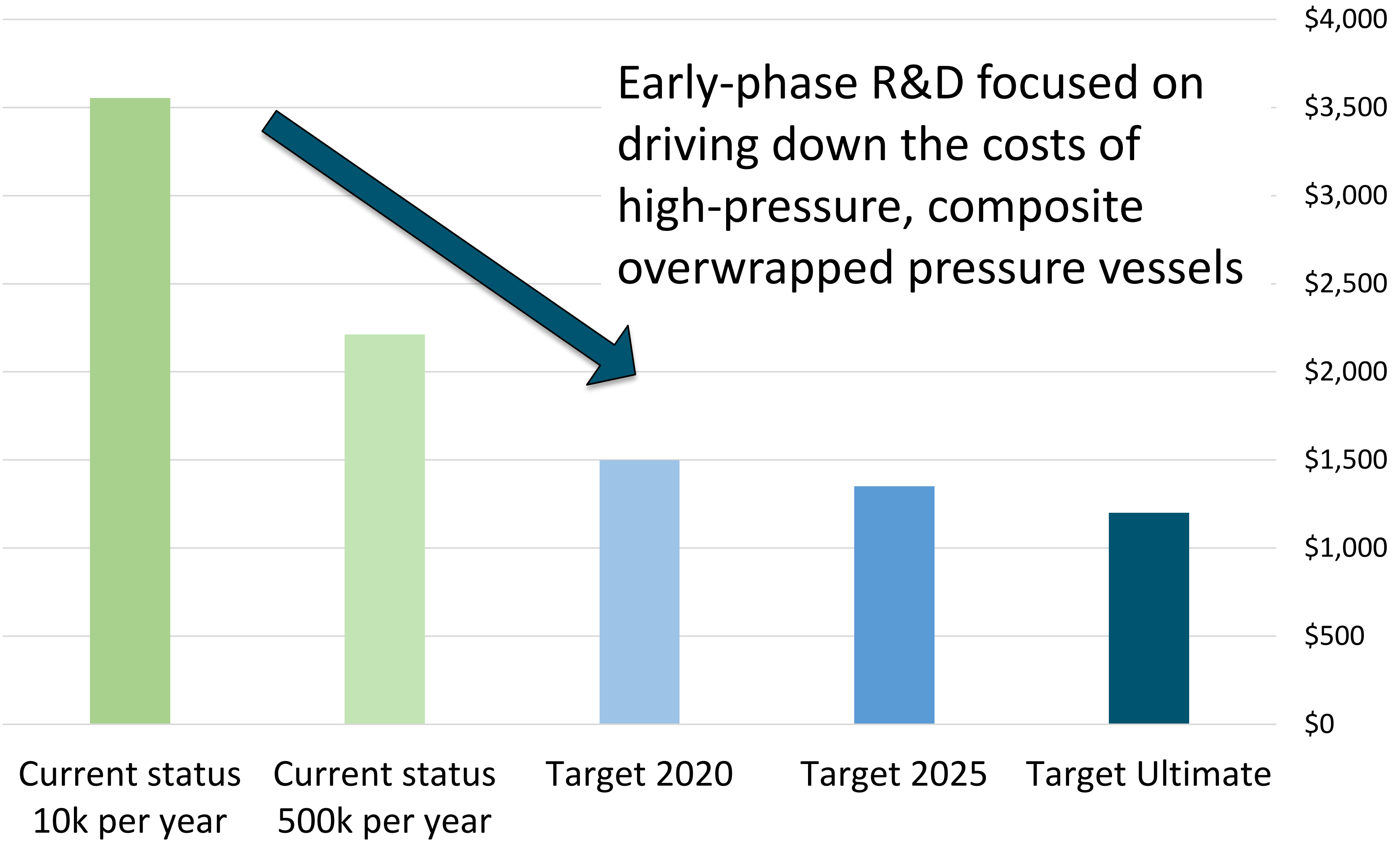
Enabling **twice the energy density** for onboard H_2 storage

Hydrogen Carriers (off-board)

In support of H2@Scale Activities

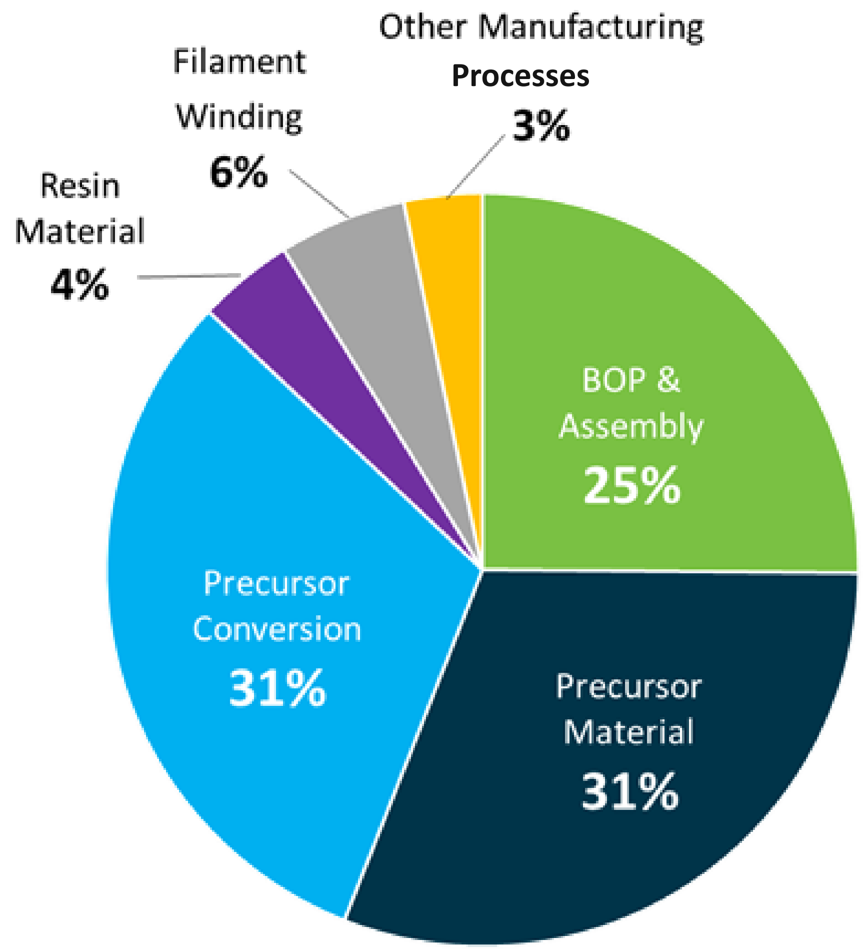
H2@Scale
U.S. Department of Energy

Challenge – Near-term – System Cost



Current Status – 700 Bar System Cost Breakout

- **Cost breakdown** at **500k systems/yr.**
- System cost is **dominated**, 72%, by **composite materials and processing**
- Carbon Fiber composite cost:
  - ~ 50% Carbon fiber precursor
  - ~ 50% Precursor fiber conversion
- BOP costs are a major cost contributor, especially at low annual production volumes

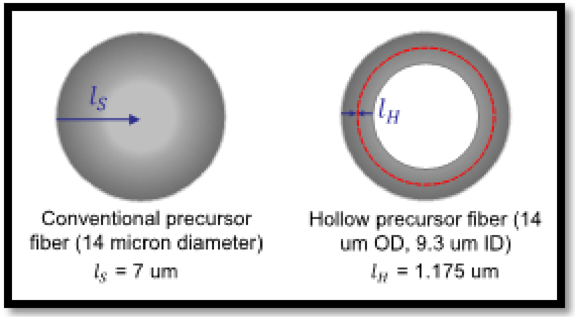


Ordaz, G., C. Houchins, and T. Hua. 2015. "Onboard Type IV Compressed Hydrogen Stora -
Cells Program Record, https://www.hydrogen.energy.gov/pdfs/15013_onboard_storage_performance_cost.pdf, accessed 5 July 2016.

Progress - Low-cost precursors efforts

University of Kentucky
[ST146]

Lower cost processing and higher specific strength - hollow PAN fibers

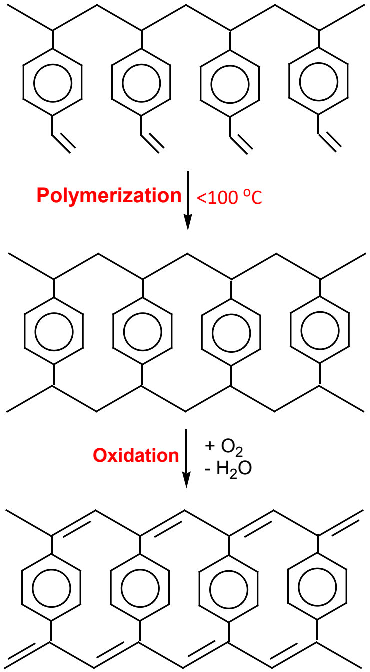


Oak Ridge Nat. Lab.
[ST148]

Lower cost processing – Melt-spun PAN fibers with ionic liquid plasticizers

Penn State University
[ST147]

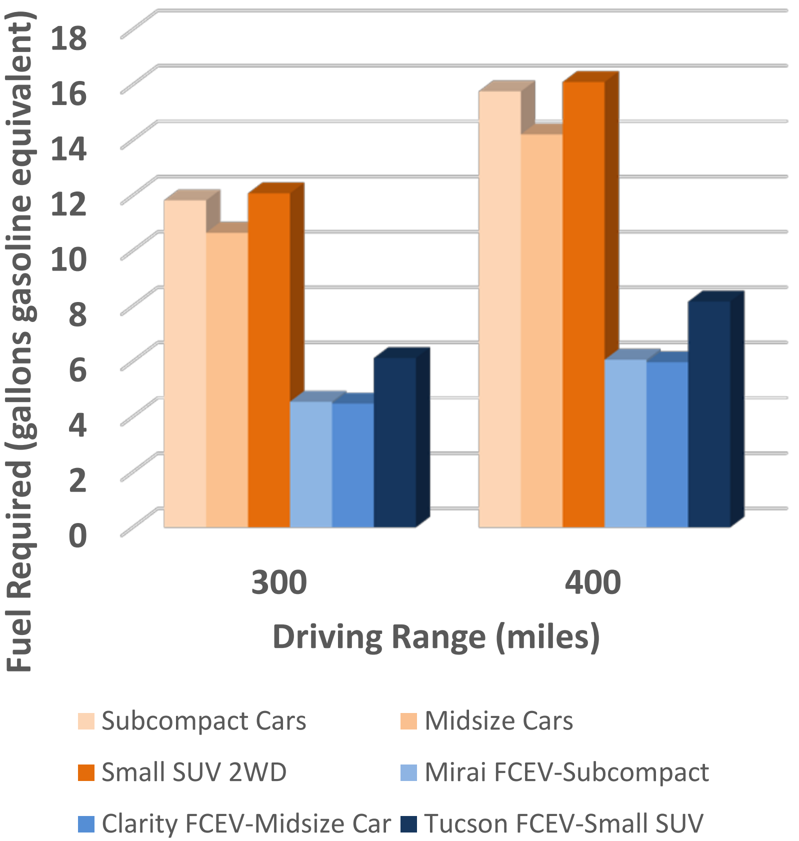
Lower cost materials – Polyolefin fibers



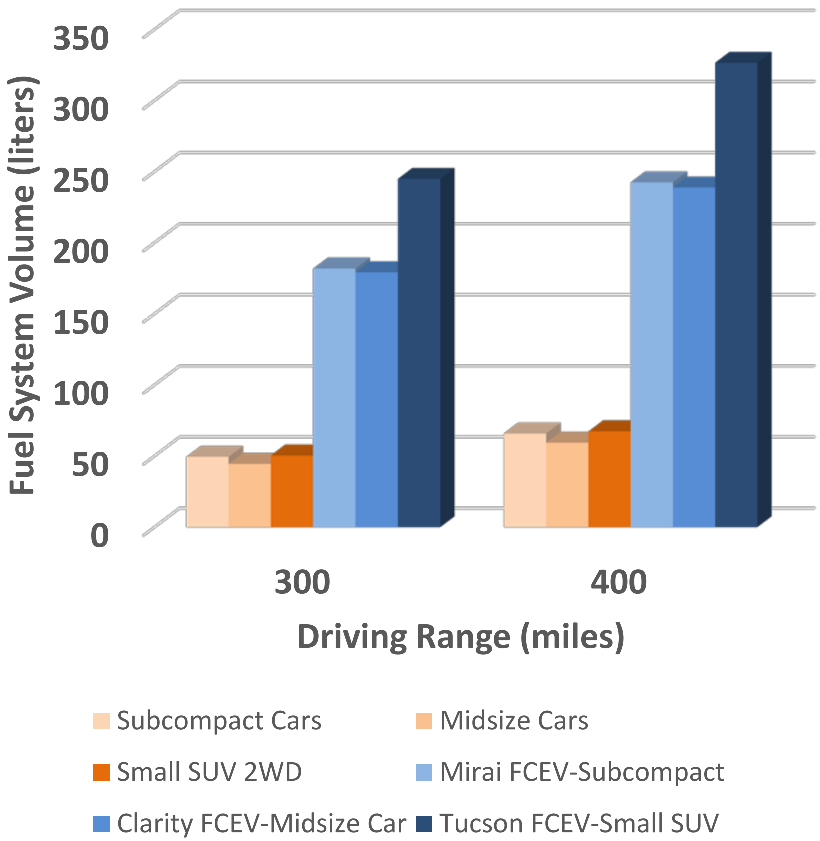
Initiated 3 new projects targeting lower cost precursors for high tensile-strength carbon fiber

Comparing Fuel Economy and Fuel System Volume

Fuel required (gge) vs range



Fuel volume (liters) vs. range



Based on EPA combined fuel economy for 2017 model year fleet averages; H_2 stored at 700 bar

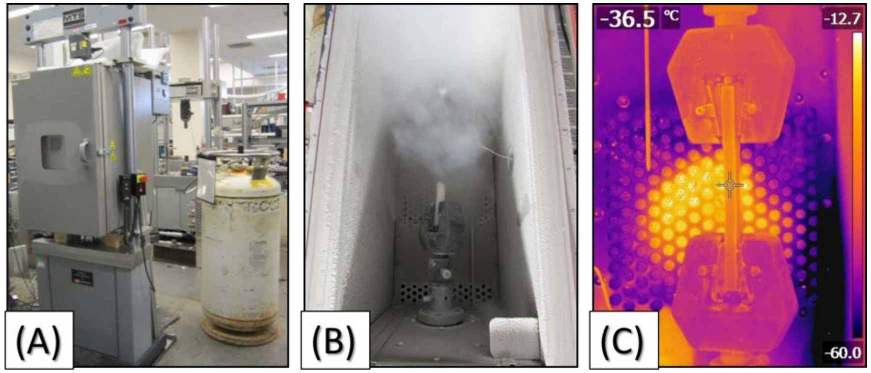
data source: www.fueleconomy.gov

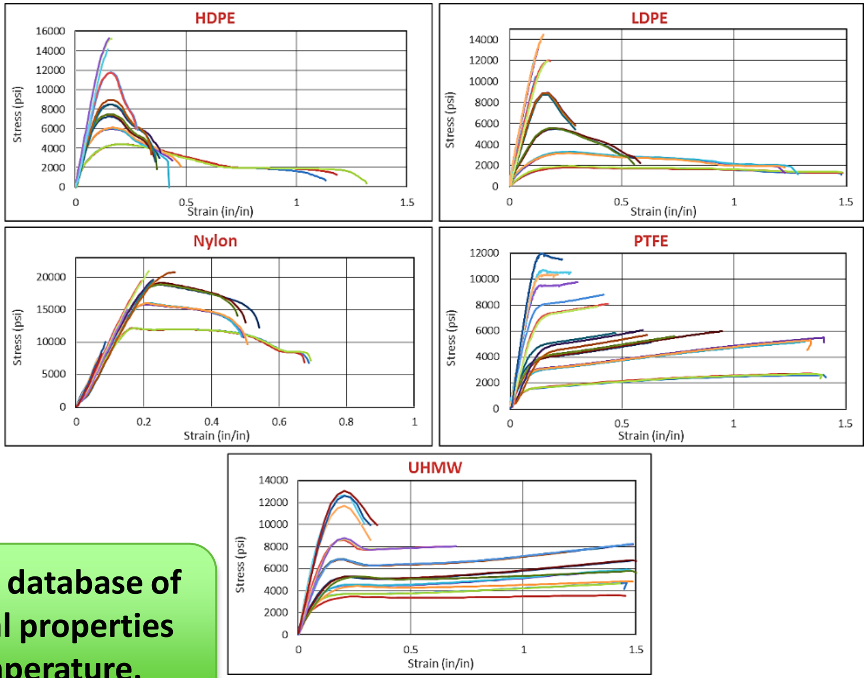
Challenge to increase the energy density of H_2 storage systems to compete with gasoline

Approach – Materials compatibility for cryogenic H_2 storage applications

New effort led by PNNL

- Develop methods and technologies to test, evaluate, and rapidly screen materials for use in pressurized cryogenic hydrogen storage applications and accelerate the pathway to tank qualification
- Test cryogenic material properties to provide input to predictive burst test models for high pressure cryogenic hydrogen pressure vessels





Develop material testing protocols and database of cryogenic material properties. Material properties can be significantly impacted by temperature.

SCS026

Approach - HyMARC – *accelerating development of storage materials and hydrogen carriers*

HyMARC

Hydrogen Materials Advanced Research Consortium

Enabling twice the energy density for hydrogen storage

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Sandia National Laboratories

BERKELEY LAB

Lawrence Livermore National Laboratory

Pacific Northwest NATIONAL LABORATORY

NIST Center for Neutron Research

SLAC NATIONAL ACCELERATOR LABORATORY

OAK RIDGE National Laboratory

Individual Seedling Projects

UMSL

Argonne NATIONAL LABORATORY

LiOx

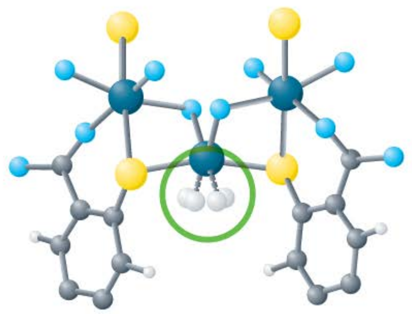
UNIVERSITY OF MICHIGAN

NREL

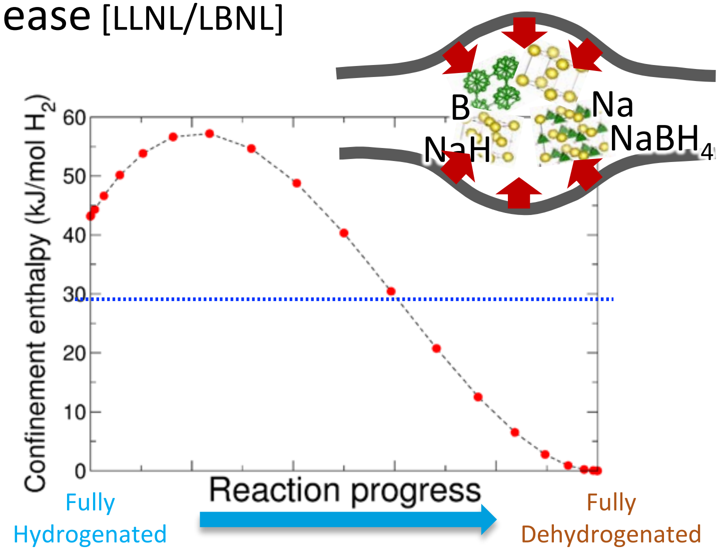
NREL

Accomplishment – HyMARC lab team [ST127-ST133]

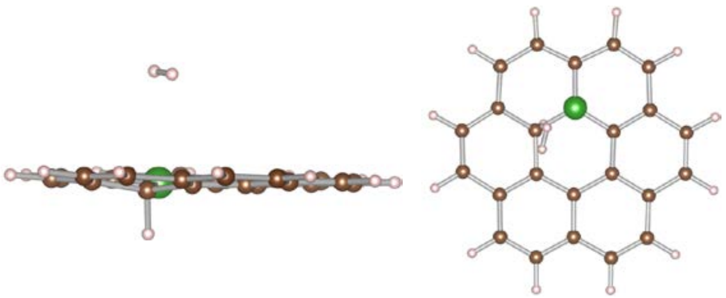
Demonstrated multiple H_2 molecules coordinated to a metal center in a MOF [LBNL/NIST]



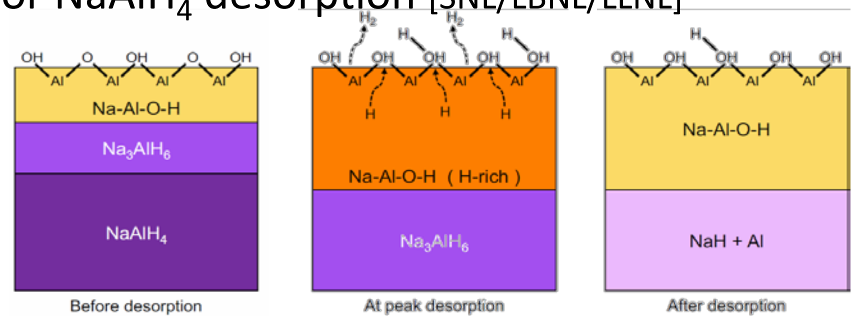
Quantifying the impact of confinement stress on thermodynamics and kinetics of hydrogen uptake and release [LLNL/LBNL]



Re-evaluated impact of boron doping on isosteric heats of adsorption in porous carbons [PNNL/NREL]

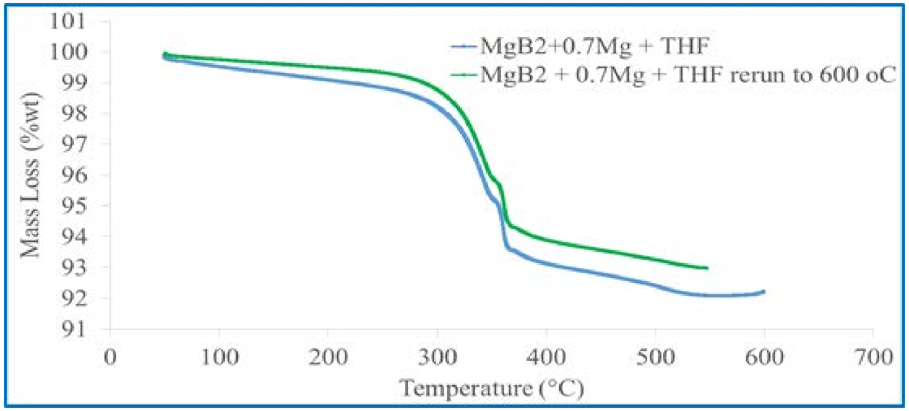


Elucidating the sorption mechanisms for complex hydrides – Ti plays no surface role, however oxides do for $NaAlH_4$ desorption [SNL/LBNL/LLNL]

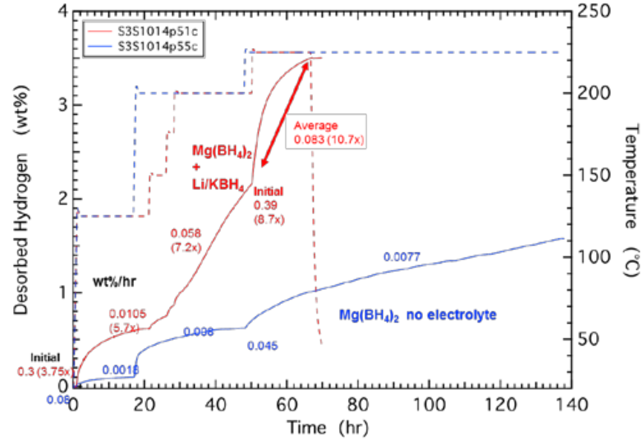


Accomplishment – HyMARC seedling projects

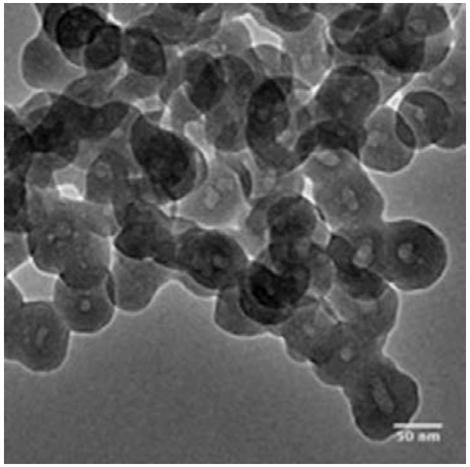
Demonstrated hydrogenation of MgB_2 to $Mg(BH_4)_2$ at 25% lower temperature and 22% lower pressure than prior state-of-the-art [UH – ST138]



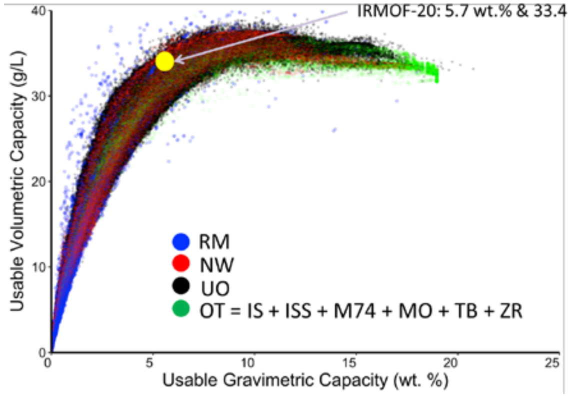
Demonstrated 10x improvement in dehydrogenation kinetics for $Mg(BH_4)_2$ [Liox – ST137]



Demonstrated ability to form Al_2O_3 coating on $Mg(BH_4)_2$ nanoparticles with improved reversibility and kinetics [NREL – ST143]



Identified >69k MOFs with potential to outperform MOF-5 through computational machine learning algorithms [UM – ST144]



Thank you from the Hydrogen Fuel Team

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

QUESTIONS?