

# H<sub>2</sub> Fuel R&D Overview

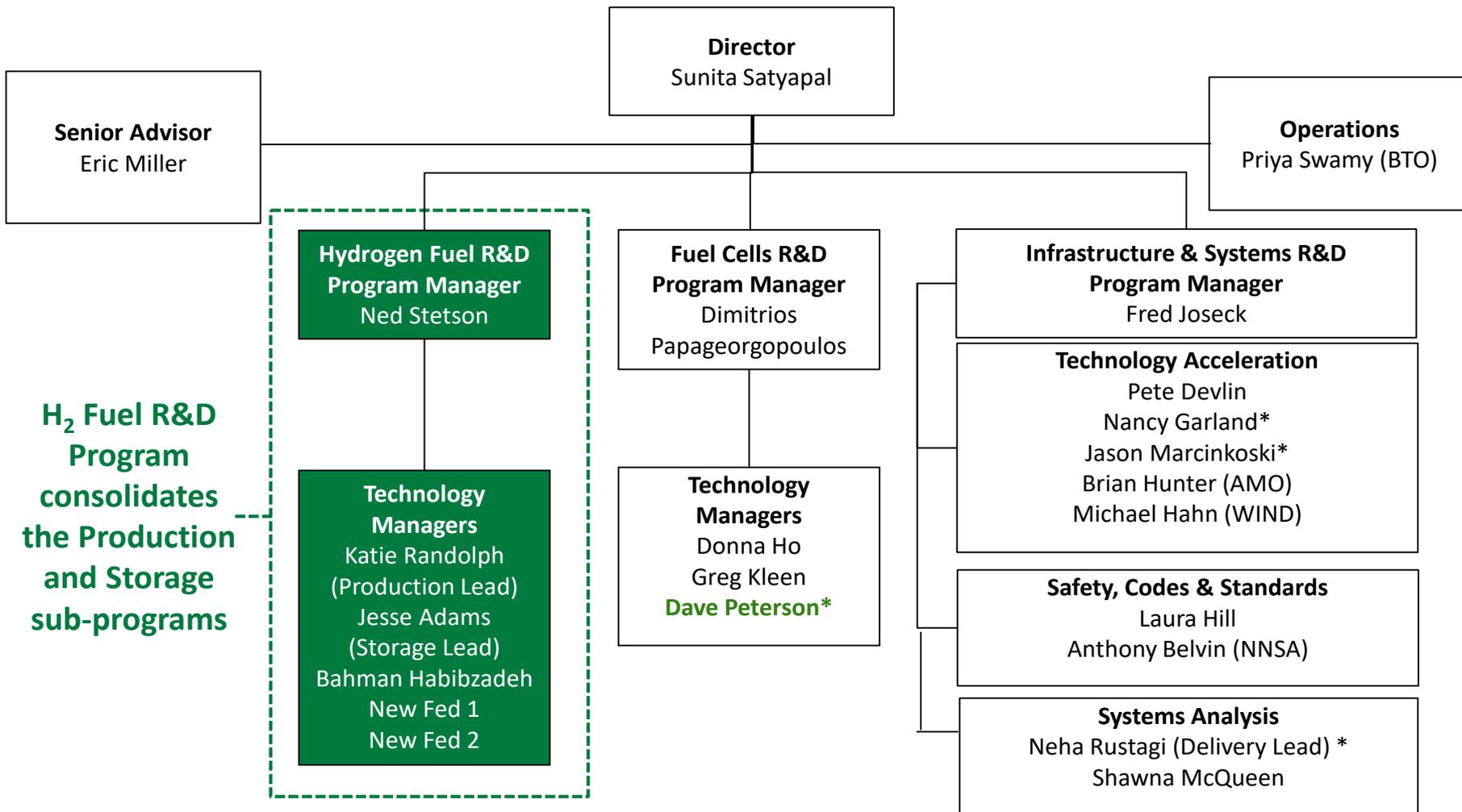
Ned Stetson, Hydrogen Fuel R&D Program Manager

2019 Annual Merit Review

April 29, 2019



# What's New in FY 2019: Organization



\* Supports multiple Program areas

# Priorities

## Hydrogen Production



### Research and Development

- Fossil fuels, biomass and waste
- Water electrolysis
- Solar water splitting
- Co-production of value-added products



### Ultimate Goal

**Less than \$2/kg**  
utilizing diverse, domestic feedstocks



### Collaboration through Consortia



**HydroGEN**  
Advanced Water Splitting Materials

Advanced water-splitting materials

**Innovative Concepts**

Ex.: Leveraging biomass/waste for H<sub>2</sub> production

## Hydrogen Storage



### Research and Development

- Low-cost storage technologies
- High-capacity materials-based storage technologies
- Cost effective transport bulk storage and technologies, enabling H<sub>2</sub>@Scale



### Ultimate Goal

**Less than \$8/kWh**  
for onboard storage



### Collaboration through Consortia



Enabling twice the energy density for onboard H<sub>2</sub> storage



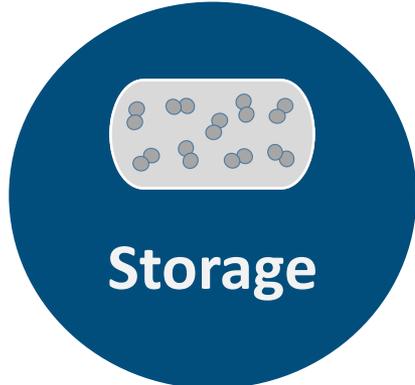
R&D investigating materials for use in cryogenic hydrogen applications

# Objectives



## Production

Low-cost, highly efficient technologies for **hydrogen production from diverse domestic resources** for both centralized and distributed production applications



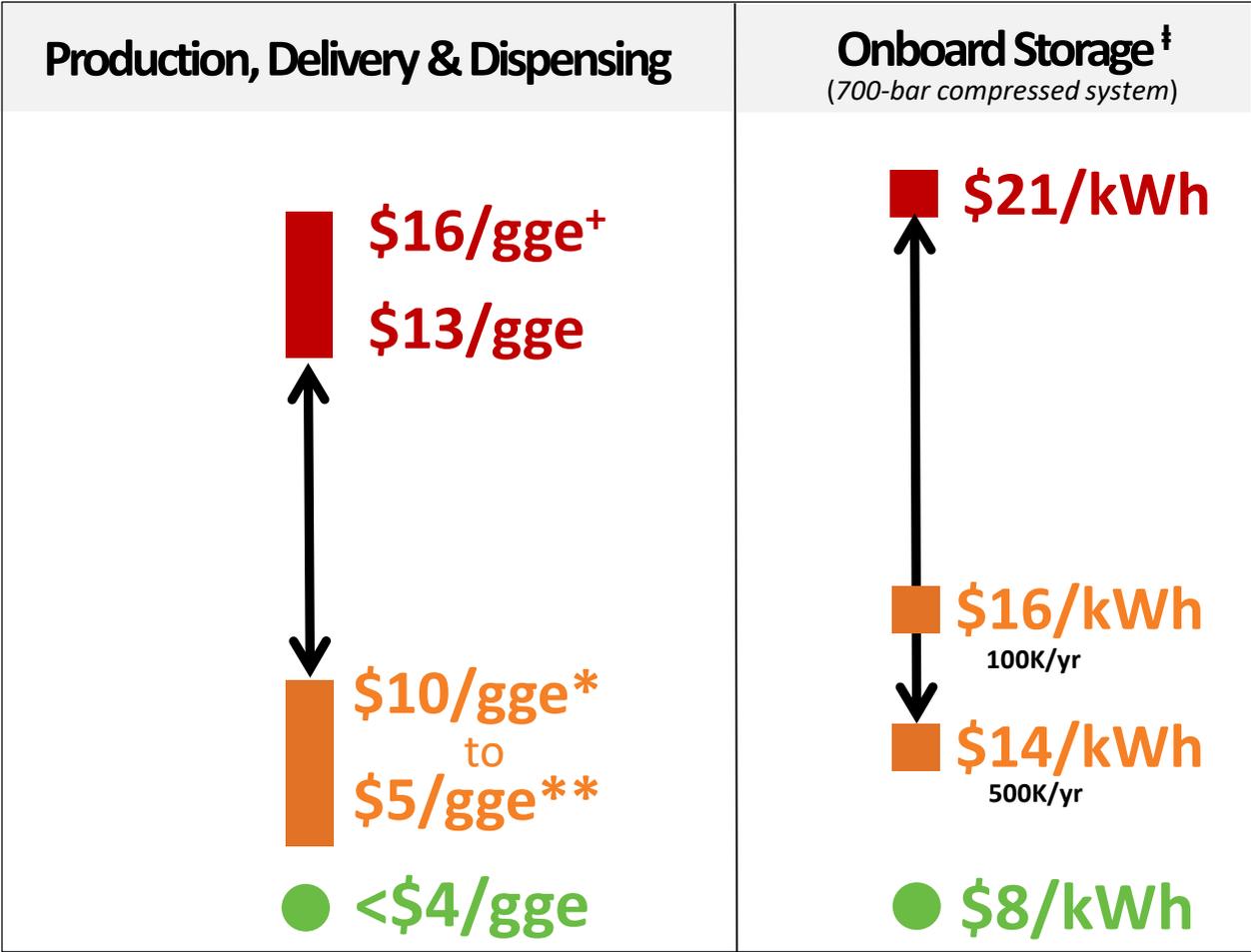
## Storage

Innovative, low-cost, and energy dense **hydrogen storage technologies for light and heavy-duty transportation and stationary applications**, including niche areas, such as energy storage, portable power and material handling equipment

**Early-Stage R&D in H<sub>2</sub> Fuel Portfolio helps enable**



# Cost Targets and Status

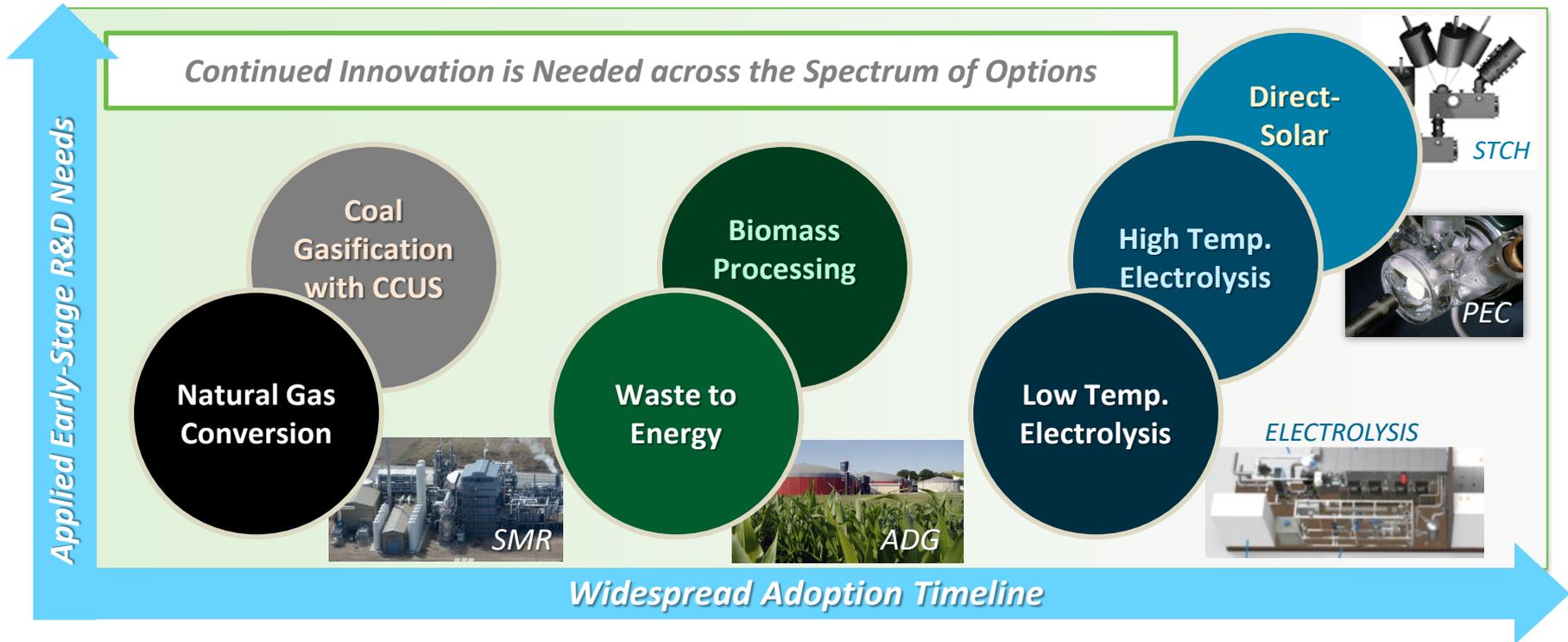


† Range assumes current production from NG and delivery and dispensing  
 \* Highest possible cost at high vol., assumes H2 from electrolysis at \$5/gge and delivery via pipelines and liquid tankers at \$5/gge  
 \*\* Lowest possible cost at high vol., assumes H2 from SMR at \$2/gge and delivery via tube trailer at \$3/gge  
 † Storage costs based on preliminary 2019 storage cost record

● **Ultimate Targets**     
 ■ **High-Volume Projection**     
 ■ **Low-Volume Estimate**

Notes: Graphs not drawn to scale and are for illustration purposes only. gge: gallon of gasoline equivalent

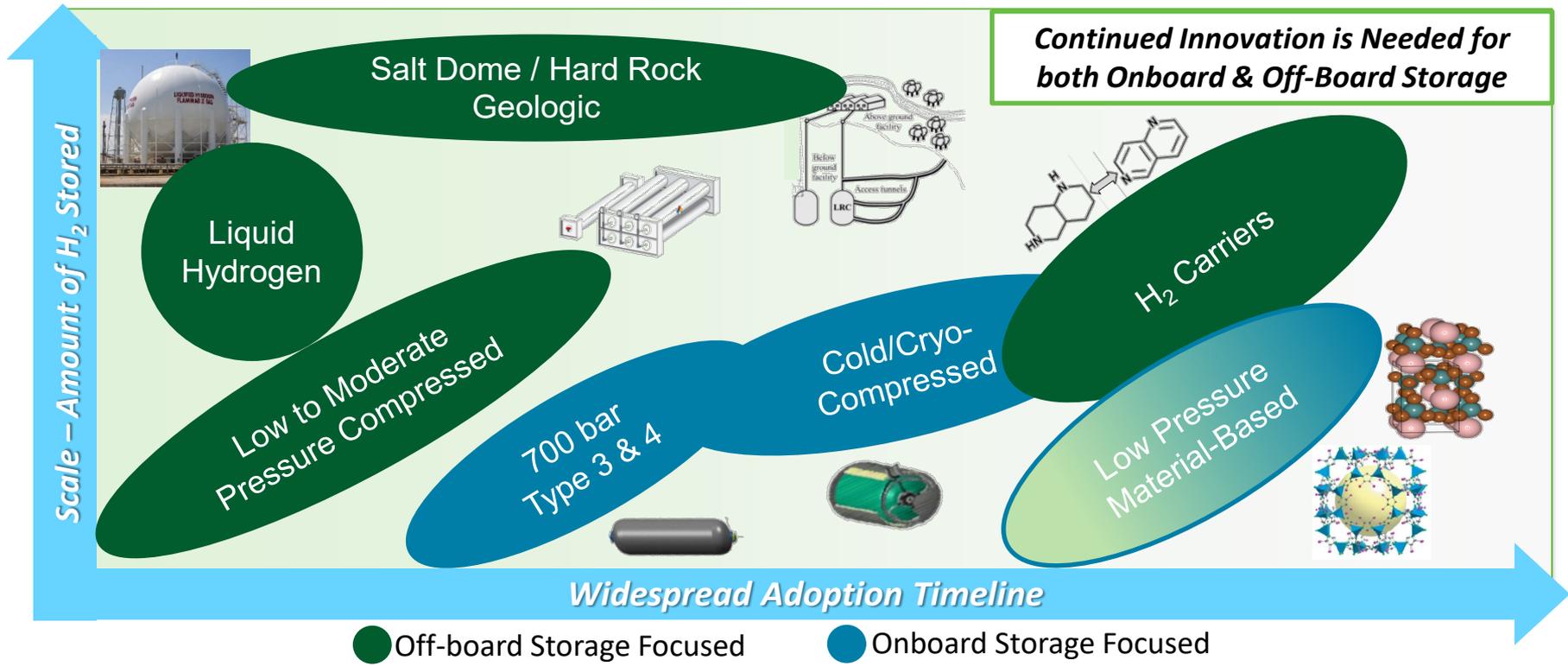
# Strategies: H<sub>2</sub> Production R&D



- ### Innovative Concepts: Fossil Fuels/Waste/Biomass
- Natural gas and coal conversion with options for CCUS and value-added byproducts
  - Industrial and biomass waste conversion providing clean-up value
  - Biogas reforming, fermentation, & other innovative concepts

- ### Advanced Water Splitting (AWS)
- Low temperature electrolysis, both grid and off-grid
  - High-temperature electrolysis, including integration with nuclear and solar
  - Emerging direct solar options, including solar thermochemical and photoelectrochemical

# Strategies: H<sub>2</sub> Storage R&D



## Off-Board Focus Areas

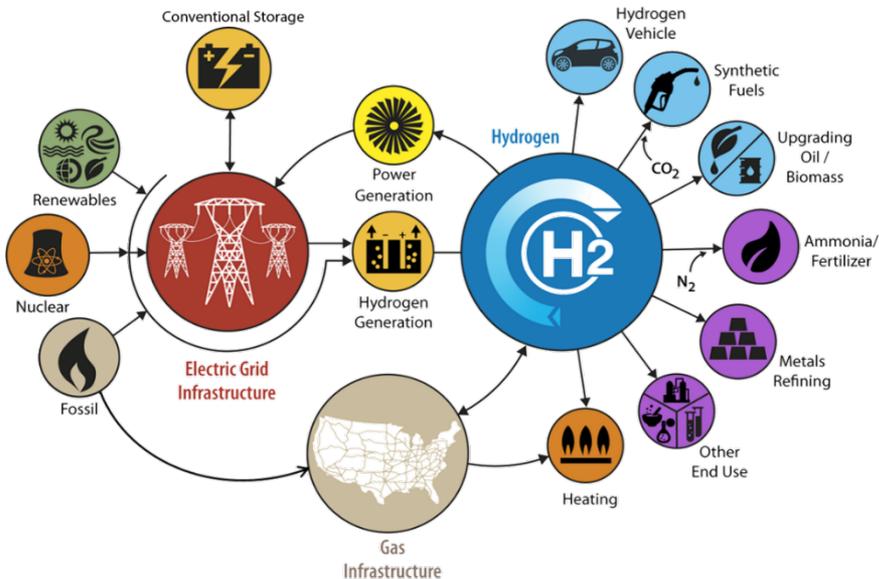
- H<sub>2</sub> carriers that provide advantages for bulk storage and transport
- Baseline bulk storage analysis to understand needs and identify technology gaps
- Improved safety, reliability, and cost

## Onboard Focus Areas

- Low-pressure, near-ambient temperature material-based storage
- Materials with improved capacity, kinetics, reversibility, and cost
- Lower-cost, high-strength carbon fiber

# Addressing Priorities: 2 FOAs with H<sub>2</sub> Fuel R&D Topics

## FY 2019 H2@Scale FOA



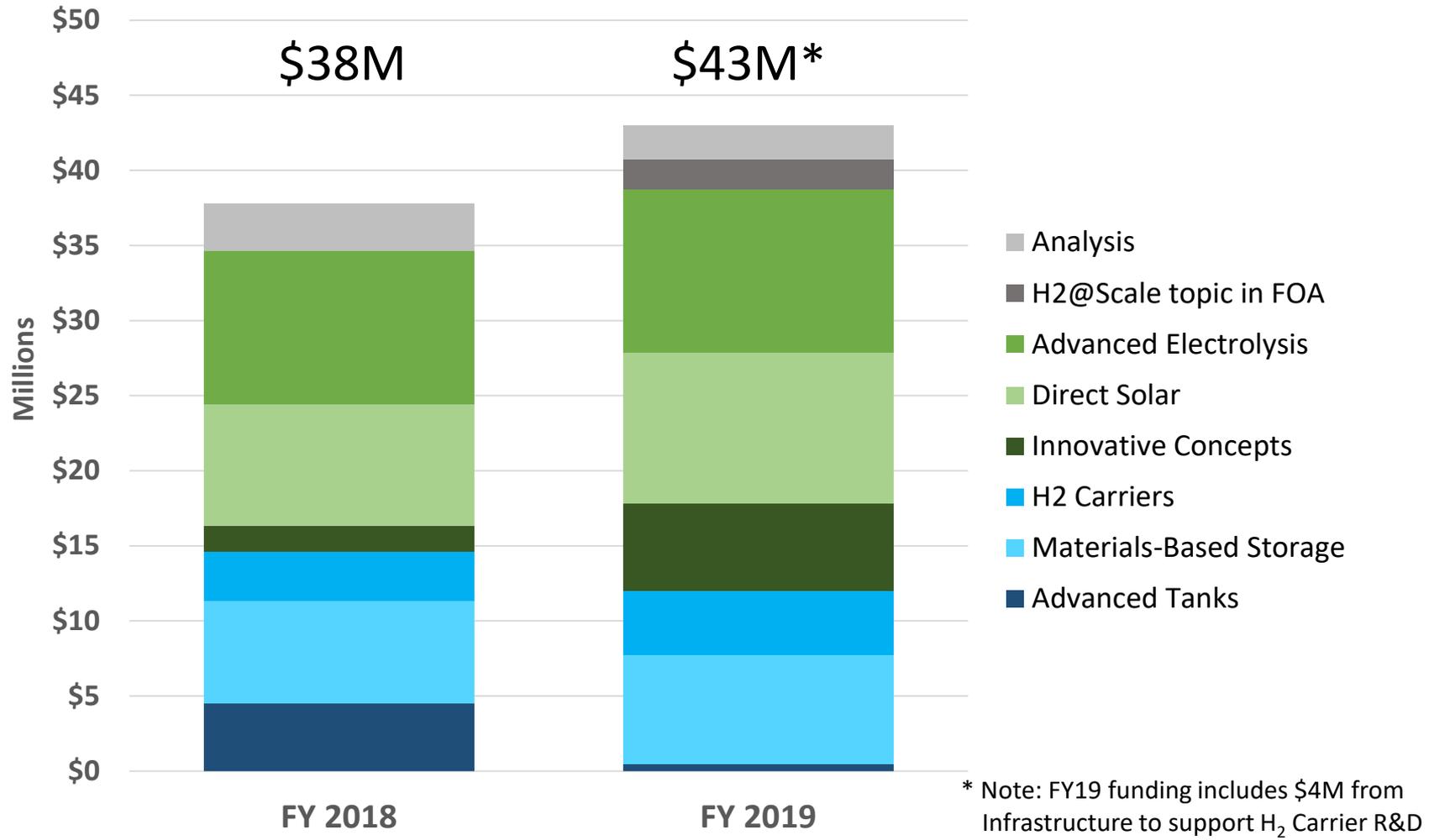
- Total funding up to \$31M
- Early stage R&D topics in storage and production include:
  - **Advanced H<sub>2</sub> storage & infrastructure R&D (\$9M)**
  - **Innovative concepts for hydrogen production & utilization (\$12M)**
  - **H2@Scale Pilot - Integrated Production, Storage, and Fueling System (\$10M)**

## FY 2019 Commercial Truck FOA

- FCTO, VTO and BETO provide combined funding of approx. \$51M
- **Total FCTO funding: \$15M**
- **Advanced storage for gaseous fuels topic included (\$3M from FCTO, \$3M from VTO)**



# Funding



**Funding distribution reflects emphasis on early-stage R&D to meet long-term targets and help enable H2@Scale**

# H<sub>2</sub> Fuel R&D project presentations

- **Hydrogen Production:**
  - Tuesday, Regency Ballroom F, 8:30 am – 6:15 pm
  - Wednesday, Regency Ballroom E, 8:30 am – 10:00 am
    - Note the change in room between Tuesday and Wednesday
- **Hydrogen Storage**
  - Wednesday, Regency Ballroom F, 8:30 am – 5:45 pm
- **H<sub>2</sub> Fuel R&D Posters**
  - Tuesday, Independence Center A&B, 6:30 - 8:00 pm

*Project presentation ID's indicated as follows:*

P100

ST100

# Consortia Approach to Address Materials Challenges in Hydrogen Fuel R&D

# H-Mat

## Early-stage R&D on hydrogen effects on polymers and metals used in hydrogen technologies

### *Collaboration across Infrastructure, H<sub>2</sub> Fuel R&D, and Safety, Codes, and Standards*

Understanding materials compatibility with hydrogen to improve reliability and cost for key technology areas



Dispensing Hoses



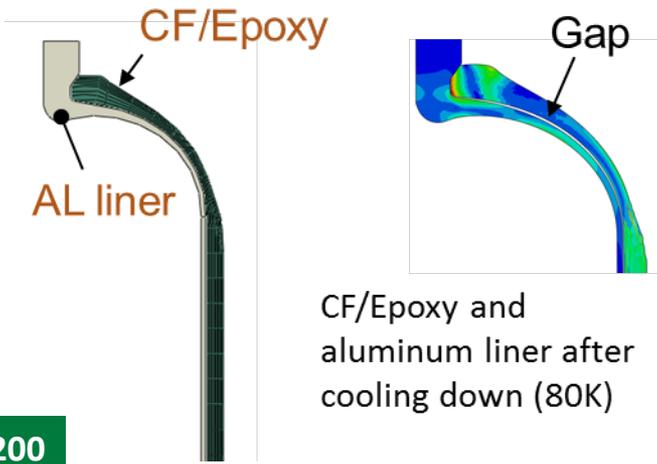
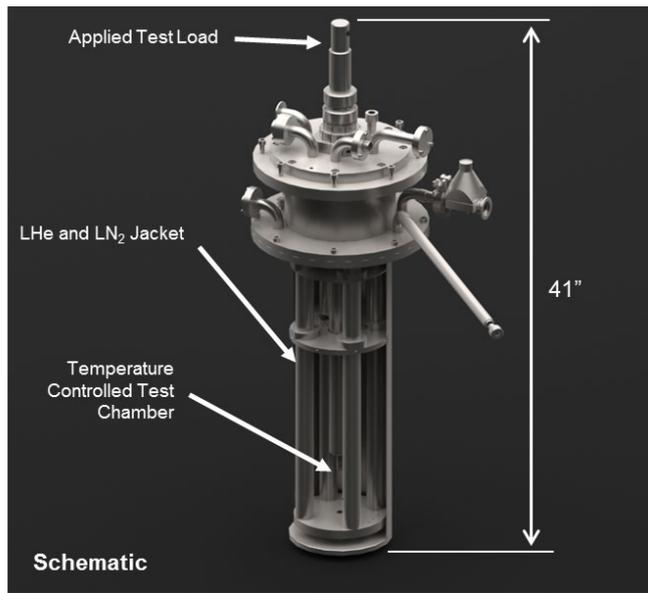
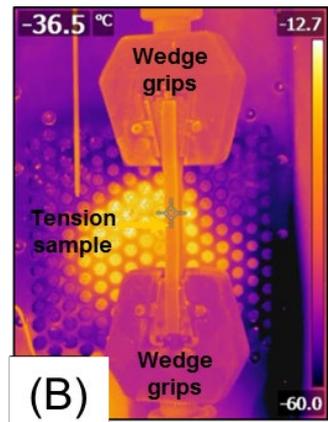
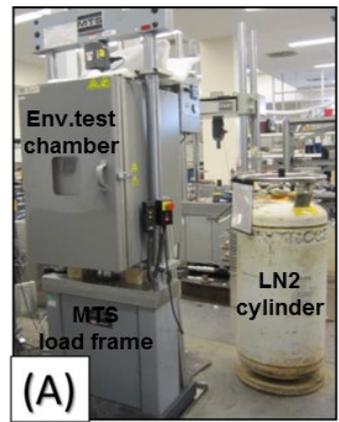
Hydrogen Storage



Hydrogen Pipelines

# H-Mat: Understanding impact of cryogenic operation on materials

Able to perform mechanical testing of metal and non-metal materials from **-253 °C to +315 °C**



Computational analysis to guide experimental research



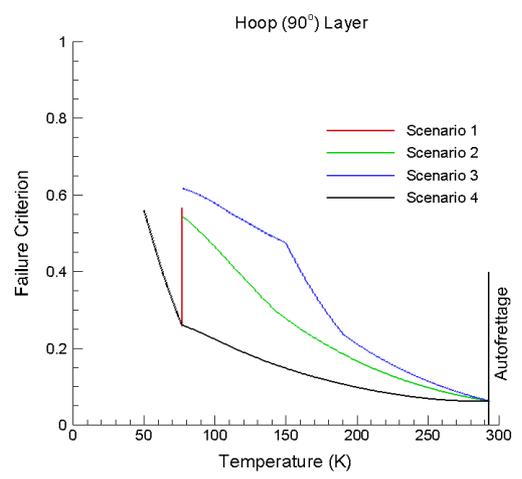
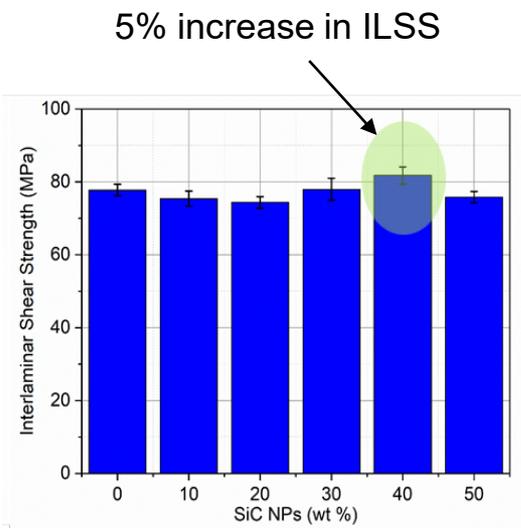
ST200

There is a need to understand the impact of thermal and pressure cycling on the performance of materials used within the hydrogen infrastructure



# H-Mat: Accomplishment Summary

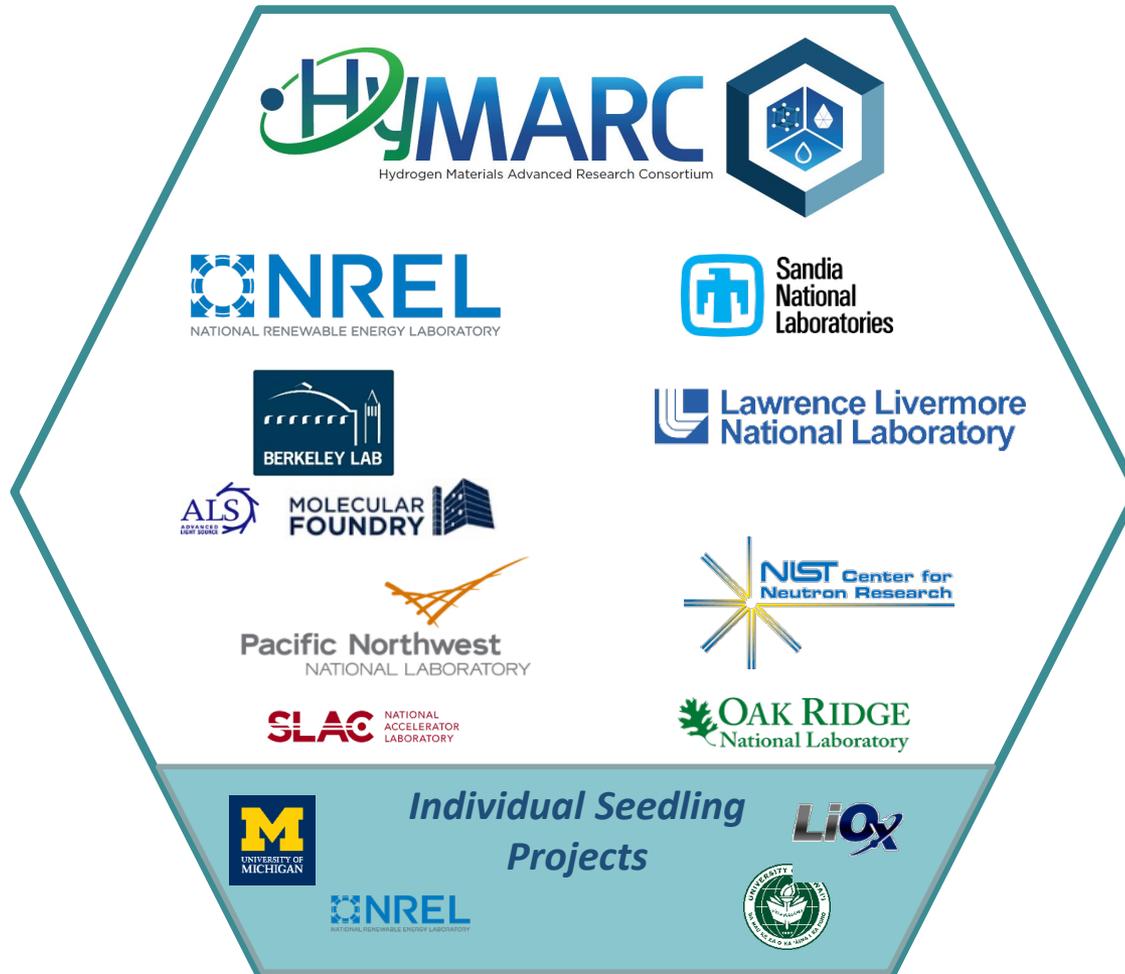
- Thermomechanical techniques for temperatures down to  $-140^{\circ}\text{C}$  proven
- 5% increase in interlaminar shear strength by nanoparticle modifications
- Approach to testing H-charged steel and aluminum materials identified
- Pressure vessel modeling assuming literature values demonstrates tank survival
- Aluminum liner strain levels are high around the neck of the tank boss



# HyMARC

# HyMARC: Accelerating the development of viable hydrogen storage materials

*Enabling twice the energy density for hydrogen storage*



## National Lab Team

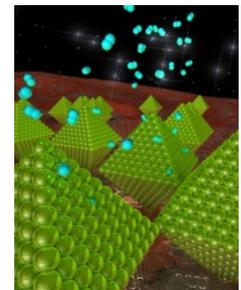
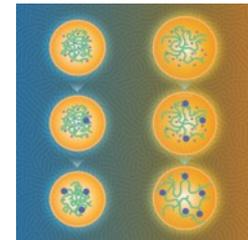
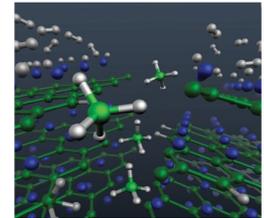
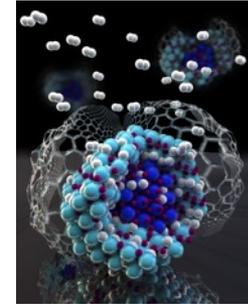
- Foundational R&D
- Computational models
- Synthetic protocols
- Advanced characterization tools
- Validation of material performance
- Guidance to FOA projects
- Database development

## Seedling Projects

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

**HyMARC Phase II successfully kicked-off,  
two separate lab teams fully integrated together into the HyMARC effort**

- **> 50 peer-reviewed journal articles published**
  - Including articles in *Nature Communications*; *Energy & Environmental Science*; *Chemical Reviews*; *Advanced Materials Interfaces*; *Advanced Functional Materials*, *Nano Letters*; *Chemistry of Materials*
  - 4 articles on journal covers
  - 2 HOT articles (in *Energy & Environmental Science*)
- 4 patents (3 issued, 1 applied)
- Numerous invited talks (major international meetings, academic, and government institutions)
- 6 Symposia and workshops organized at major conferences
- **> 20 postdocs supported**
- Global connectivity through extensive network of collaborations



See presentations ST127-ST132 for more accomplishments

# HyMARC: Phase II Task Structure



**Mark Allendorf (SNL) & Tom Gennett (NREL)  
Co-Directors**

**Task 1  
Sorbents  
Gennett**

**Task 2  
Hydrides  
Allendorf**

**Task 3  
Carriers  
Autrey**

**Task 4  
Adv. Char.**  
Parilla  
(NREL validation)  
Prendergast  
(ALS, SLAC, MF)  
Bowden  
(PNNL NMR)  
Brown  
(NIST Neutron)  
Toney  
(SLAC, X-ray)

**Task 5  
Seedling  
Support  
Allendorf  
Gennett**

**Task 6  
Data Hub  
Munch  
(NREL)**

**Focus  
Areas**

**Focus  
Areas**

**Focus  
Areas**

**Focus Areas**

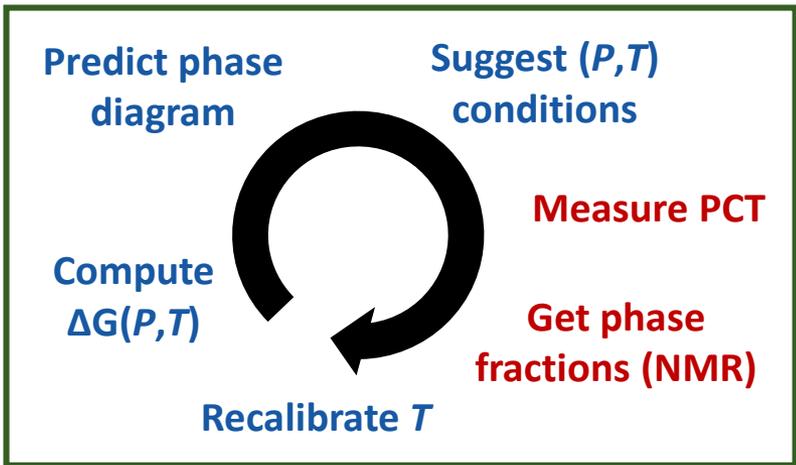
**Task leads:**  
Coordinate work  
Milestone accounting  
Reporting

**Focus Areas (new concept):**  
Multi—lab Research clusters  
Defined topic  
Dynamic, agile  
Duration: as little as 1 year  
Applied topics: Go/No-Go  
Foundational topics: milestones

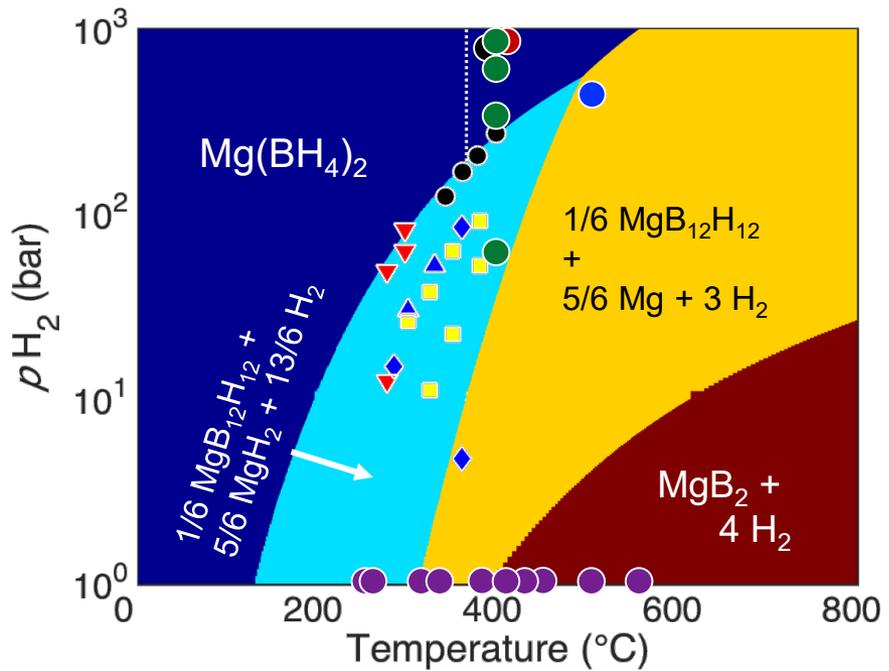
**User Facility POCs**



# HyMARC: Close coupling of computation and experiment

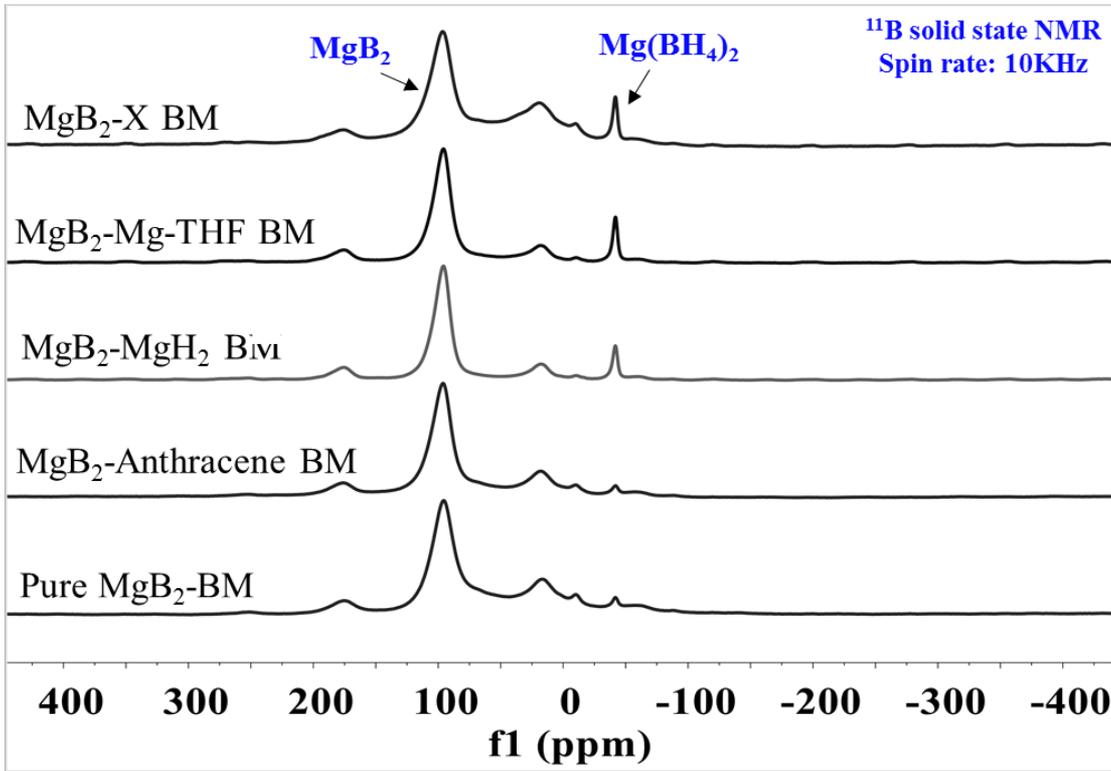
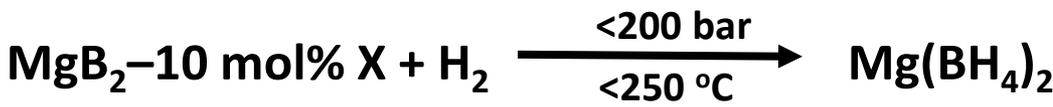


*Phase diagrams are refined through experiment-theory feedback cycle- improving accuracy*



**Example: Accurate bulk phase diagram prediction and validation**

Significant reduction in hydrogenation conditions required for  $MgB_2$   
Collaboration of University of Hawaii (seedling), PNNL, SNL, LLNL and NREL



Demonstrated formation of  $Mg(BH_4)_2$  under conditions of **less than 200 bar and 250 °C**, significantly reduced from prior 700 bar and 300 °C required conditions.

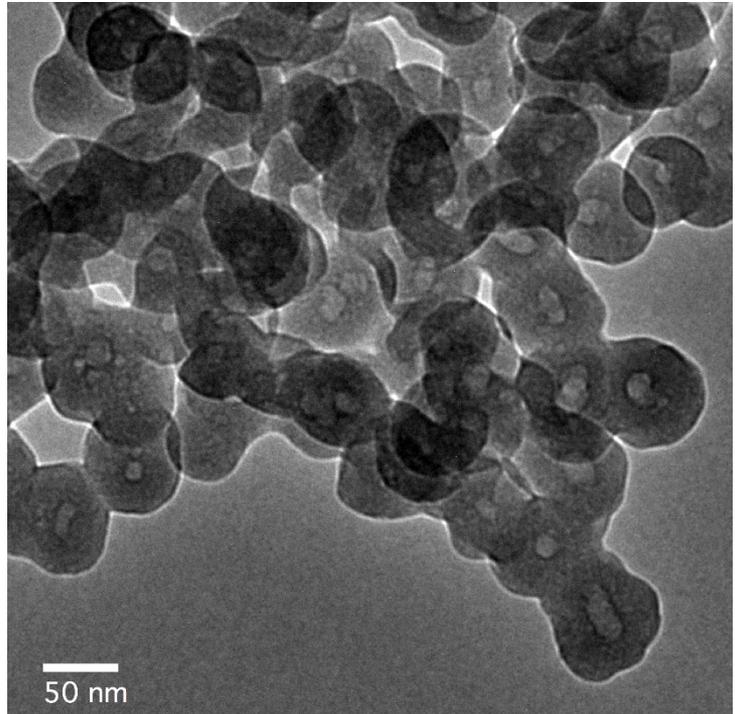
ST138

Additives are effective in reducing required hydrogenation conditions for  $MgB_2$

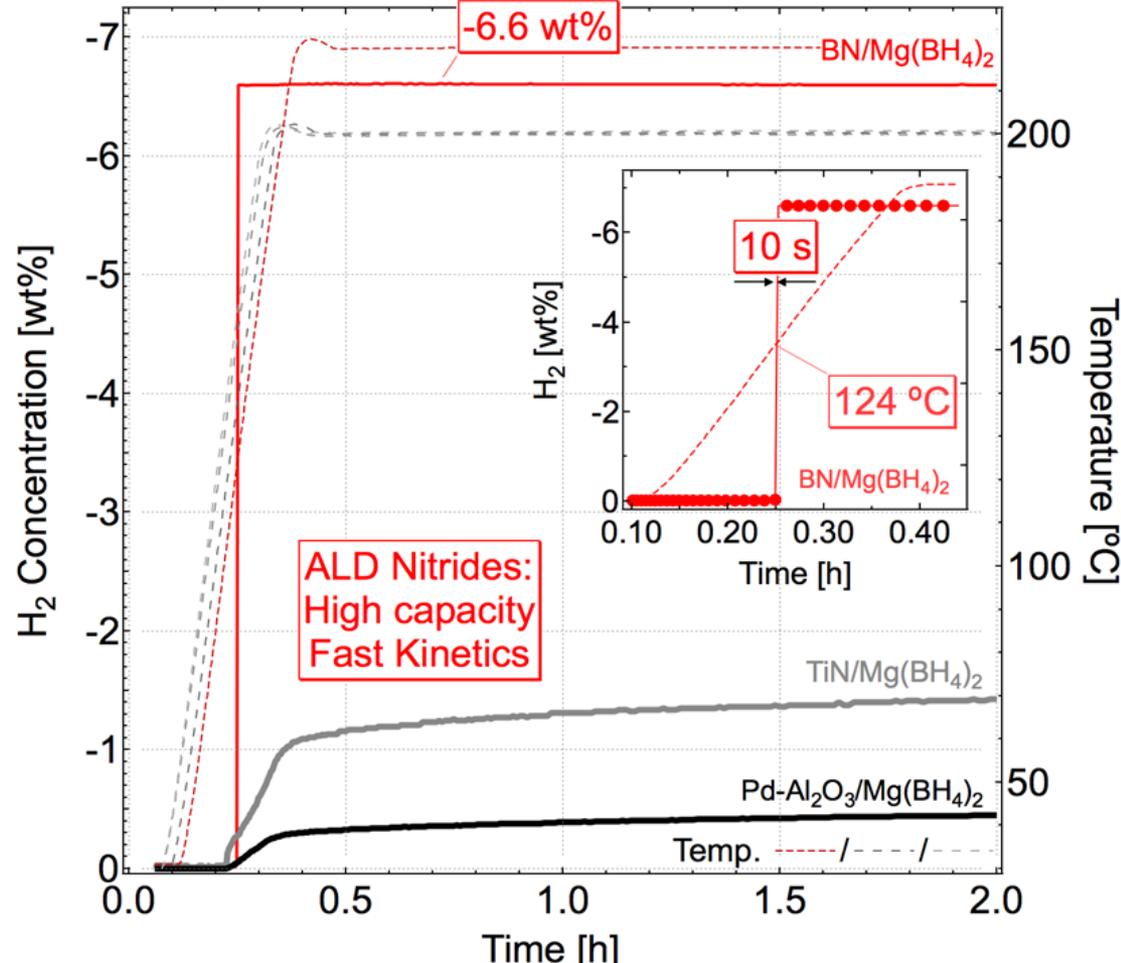
# HyMARC: Exciting new preliminary results



Atomic layer deposition (ALD) used to coat nanoparticles of  $Mg(BH_4)_2$



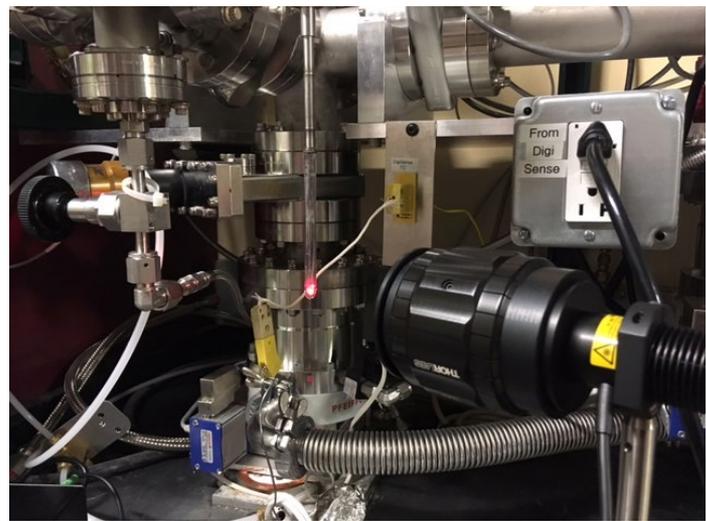
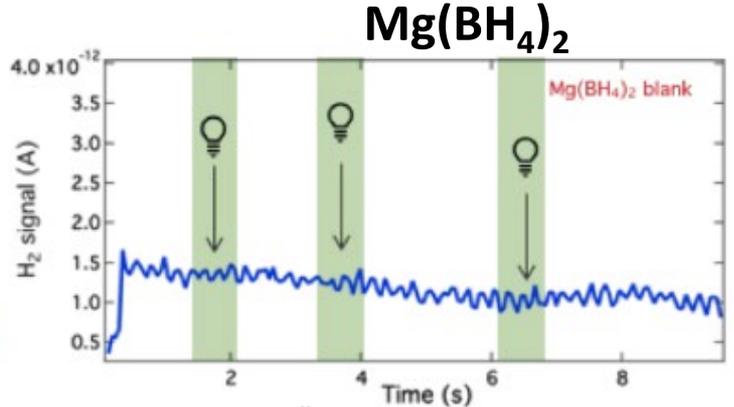
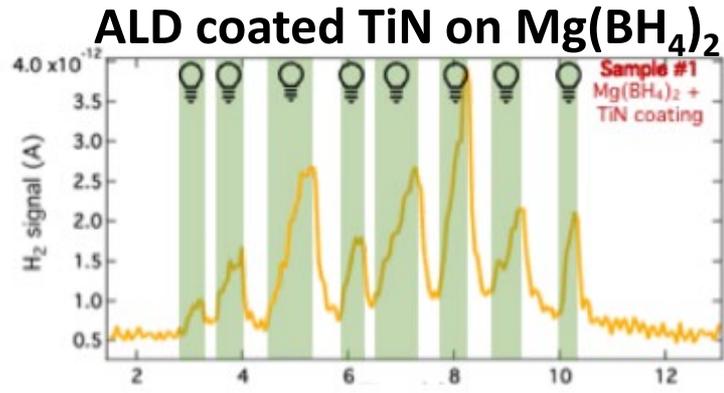
Desorption plots for nano-encapsulated  $Mg(BH_4)_2$



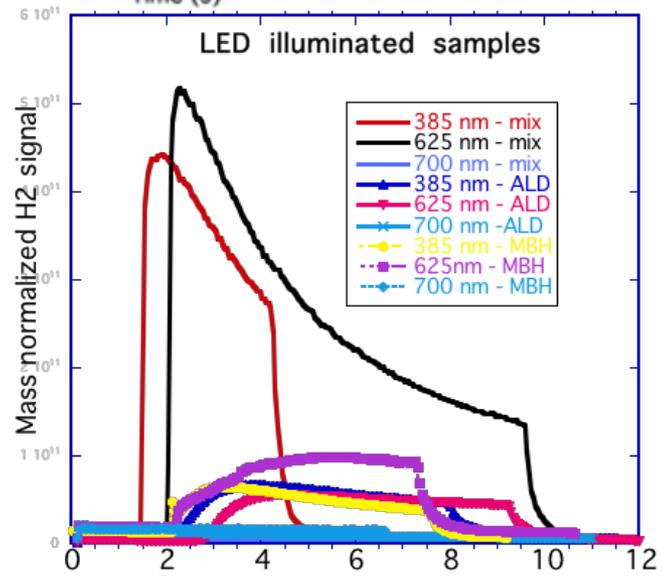
ST143

ALD nitride coated  $Mg(BH_4)_2$  nanoparticles shown to have rapid desorption kinetics at relatively low temperatures (*NREL seedling*)

## Controlled hydrogen release from $Mg(BH_4)_2$ using light! (NREL)



**500 mA LEDs:**  
**385 nm,**  
**625 nm,**  
**& 700 nm**



ST131

Plasmonic photocatalysts shown to have potential to effect room temp  $H_2$  release

# HydroGEN

# Pioneering Research in Water Splitting

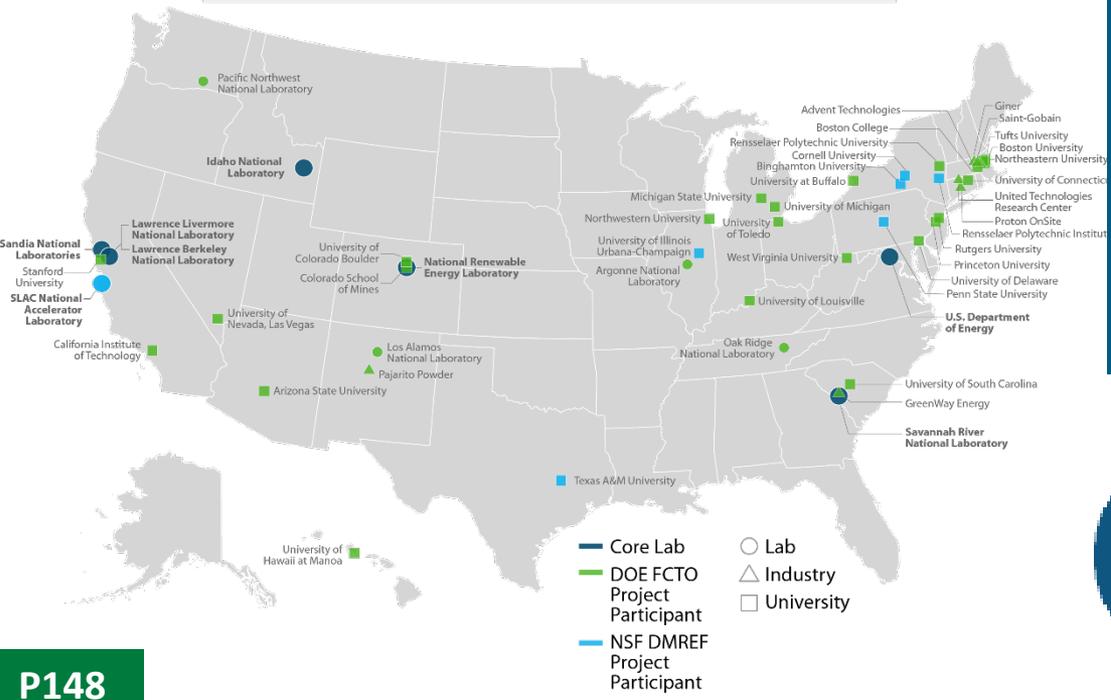


## HydroGEN

Advanced Water Splitting Materials



11 Labs    7 Companies    30 Universities    2 Funding Agencies



- 16 Successful GNG Decisions
- 2 new HTE projects
- 4 new NSF DMREF Projects
- 17 Publications
- 2 Work for Others Agreements
- 5 Data Tools; > 4000 Files; > 158 users
- Held Benchmarking Workshop
- Multiple AWS Standard Protocols



P148



# Supernodes: Innovative multi-lab framework where capability nodes & experts work synergistically to address AWSM R&D needs, gaps & problems



## ***HTE: Characterizing HTE Electrode Microstructure Evolution***

Led by INL with LBNL, LLNL, NREL and SNL—integrating 6 nodes



## ***STCH: Develop Atomistic Understanding of Layered Perovskite $\text{Ba}_4\text{CeMn}_3\text{O}_{12}$ & Polytypes***

Led by SNL with LLNL and NREL—integrating 7 nodes



## ***LTE/STCH Hybrid: Linking Materials to Electrode Properties to Performance***

Led NREL with SRNL and LBNL—integrating 8 nodes



## ***PEC: Emergent Degradation Mechanisms with Integration and Scale Up of PEC Devices***

Led LBNL and NREL—integrating 8 nodes



## ***LTE/PEC: Multiscale, Multi-Theory Modeling to Understand the Oxygen Evolution Reaction Across pH Ranges***

Led LLNL and LBNL with NREL—integrating 6 nodes



# HydroGEN: Exciting Accomplishments

## High Temperature Electrolysis

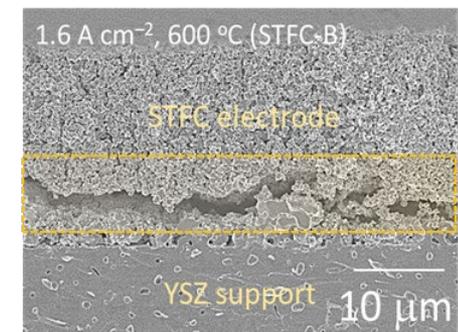
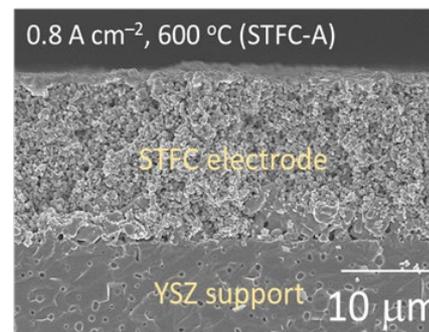
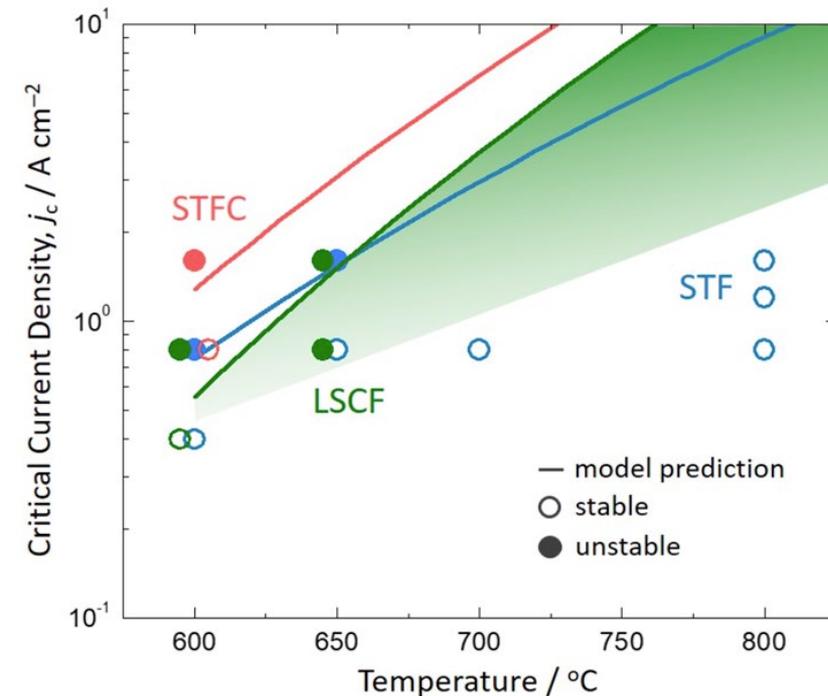
P153



Northwestern  
University

**Northwestern University developed an improved understanding of SOEC degradation mechanisms**

- Experimentally validated model predicts critical current density for fracture at electrode/ electrolyte interface with multiple materials and temperatures



**SOEC degradation advances: Decreased stack degradation and improved understanding of degradation mechanisms**

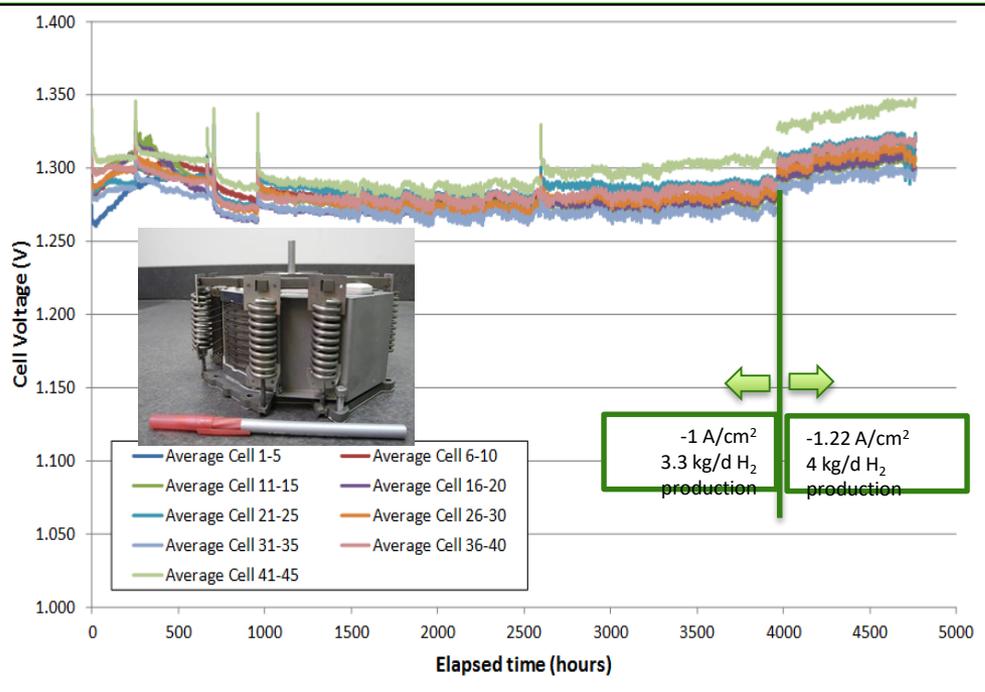
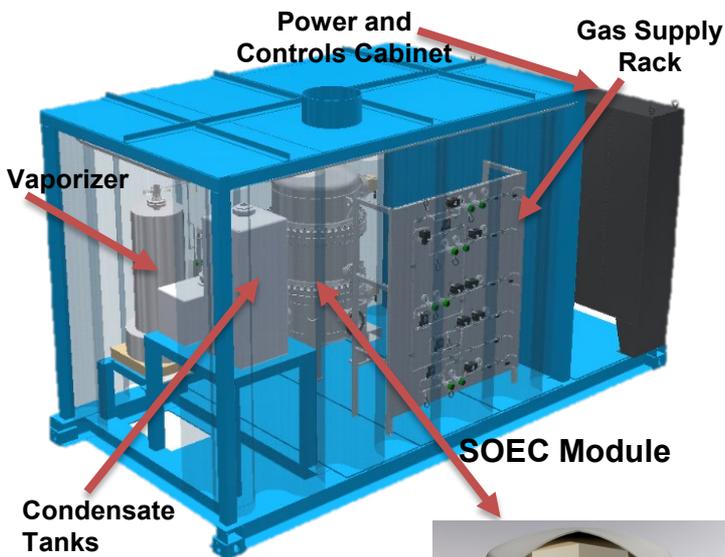
# H<sub>2</sub> Production: Exciting Accomplishments

## High Temperature Electrolysis

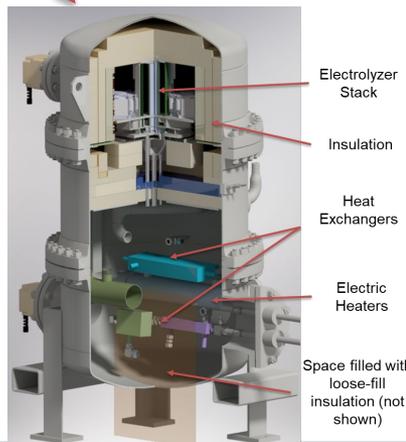
TA019



FuelCell Energy demonstrated 45 cell SOEC stack with virtually no degradation over ~4000 hr at 1 A/cm<sup>2</sup> with >95% electrical efficiency



>4 kg H<sub>2</sub>/day prototype unit designed and under construction; will be tested for >1000 hr



**SOEC degradation advances: Decreased stack degradation and improved understanding of degradation mechanisms**



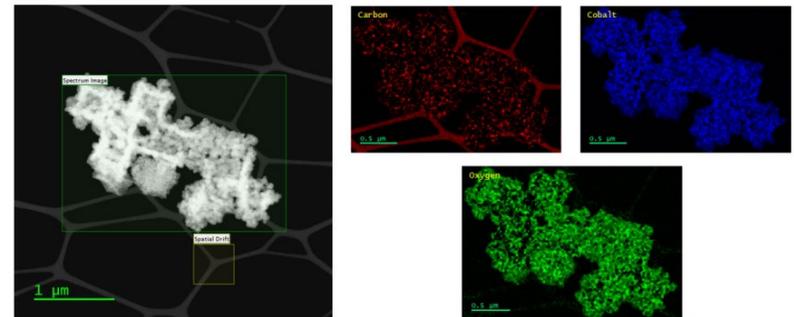
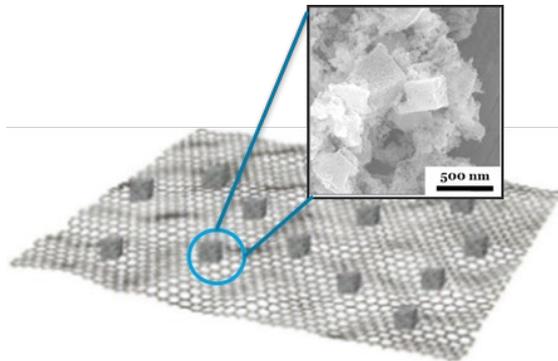
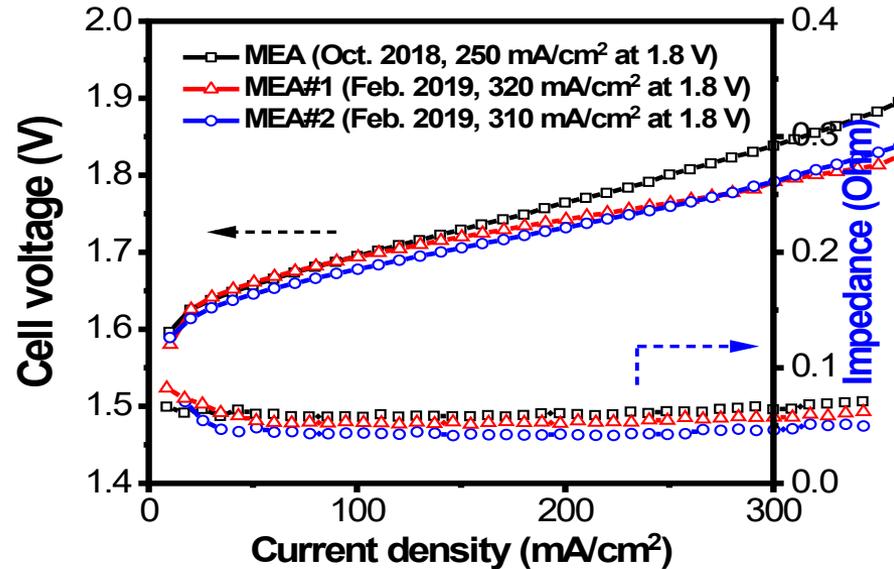
# HydroGEN: Exciting Accomplishments

## Low Temperature Electrolysis

P157

**Argonne Nat. Lab.:** One of the first MEA demonstrations of **PEM-based** water electrolysis with **PGM-free OER catalyst** at practical operating conditions

- Developed graphene-supported activated Co-MOF (Co-MOF-G-O) OER catalysts
- Achieved current density  $> 300 \text{ mA/cm}^2$  at 1.8 V (testing at Giner)



**PGM-free electrodes demonstrating reasonable current densities in MEAs at typical cell operating voltages**



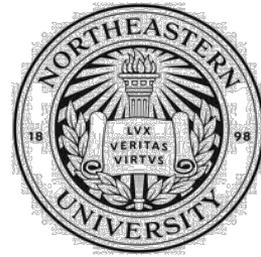
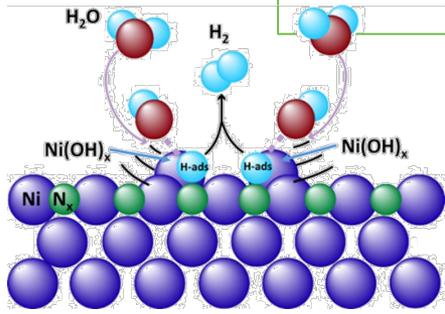
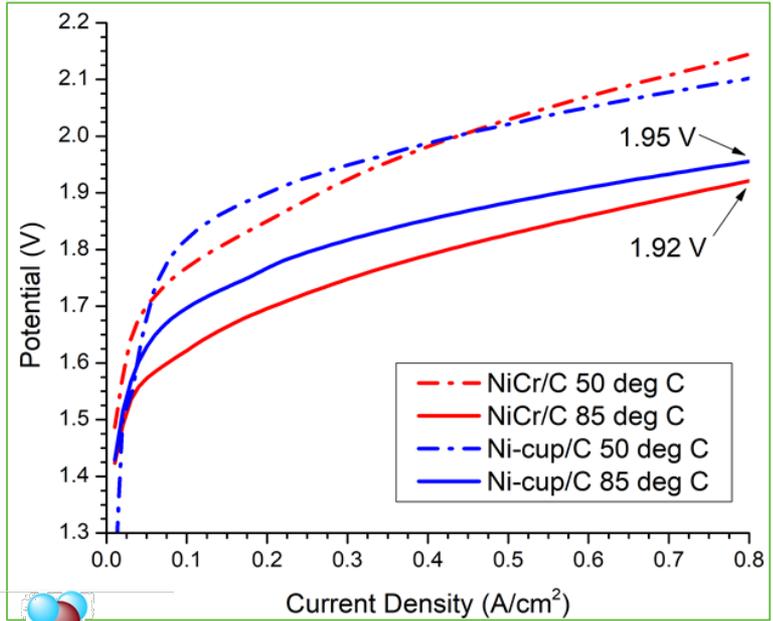
# HydroGEN: Exciting Accomplishments

## Low Temperature Electrolysis

P156

**Northeastern University** demonstrated continued performance improvement for **completely PGM-free AEM** electrolysis with advanced catalysts and membranes

- Achieved current density of 800 mA/cm<sup>2</sup> at 1.92 V
- OER catalyst - NiFe/Raney Ni
- HER catalyst - NiCr/C and Ni-cup/C
- Membrane – U. Delaware polyaryl piperidine-based AEM with high temperature stability



**PGM-free electrodes demonstrating reasonable current densities in MEAs at cell operating voltages**



# HydroGEN: Exciting Accomplishments

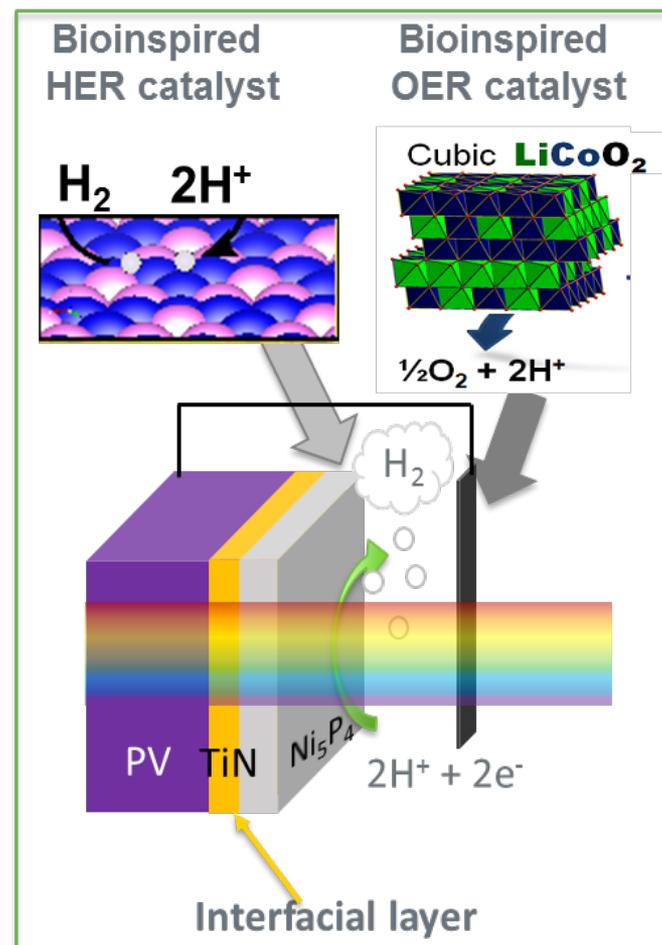
## Photoelectrochemical H<sub>2</sub> Production

P160



Rutgers demonstrated a:

- **Bioinspired** high solar-to-hydrogen efficiency system
- **11.5% with PGM-free Ni<sub>5</sub>P<sub>4</sub> HER catalyst**
- Integrated with high performing photoabsorber
- **Comparable performance** to PGM PtRu catalyst!



Replacing PEC components with low-cost,  
high performance alternatives while still achieving high STH!



# HydroGEN: Exciting Accomplishments

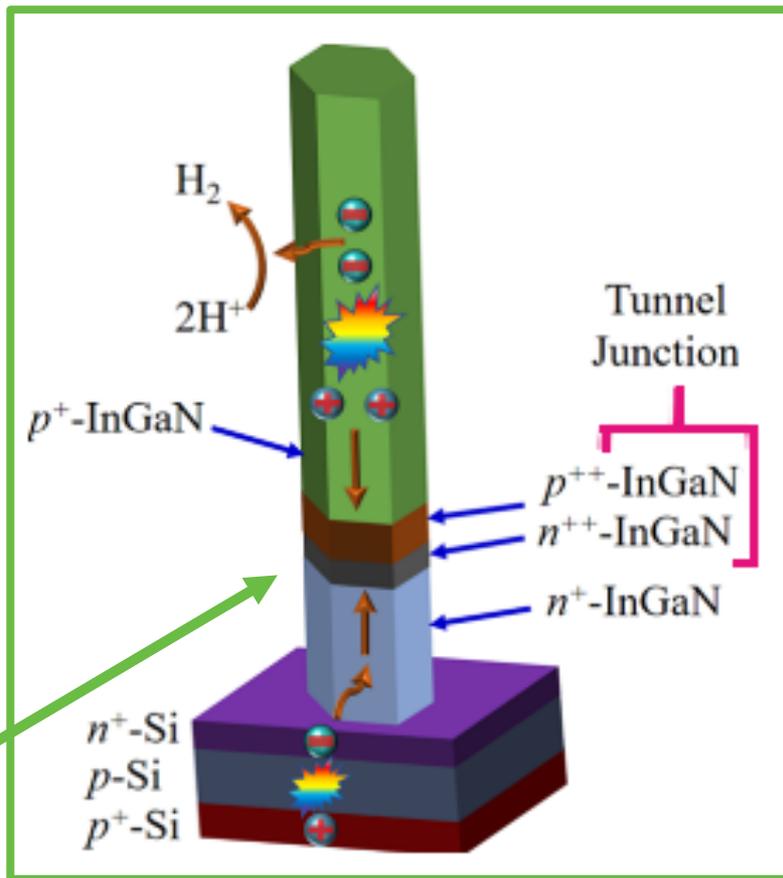
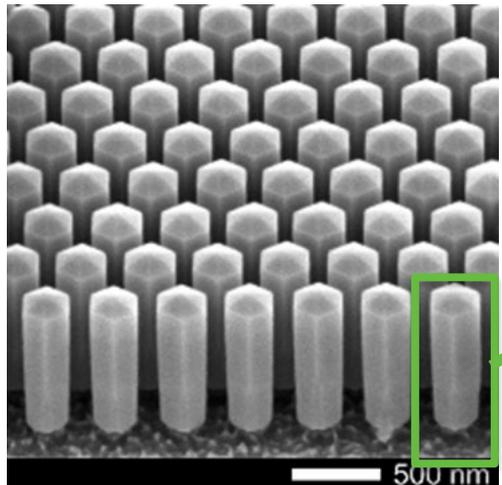
## Photoelectrochemical H<sub>2</sub> Production

P163

### University of Michigan:



- **First Si-based** double-junction photoelectrode with solar-to-hydrogen efficiency >10%
- Demonstrated GaN/Si photocathode with **stable operation for >100 hours** at high photocurrent density.



Replacing PEC components with low-cost, high performance alternatives while still achieving high STH!



# HydroGEN: Exciting Accomplishments

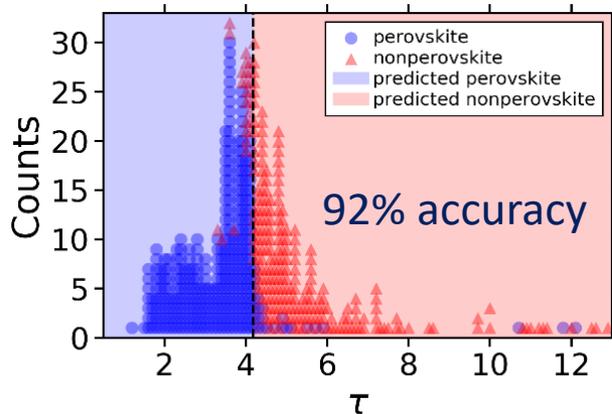
## Solar Thermochemical H<sub>2</sub> Production

**University of Colorado at Boulder:** Utilized **Machine Learning** to rapidly screen  $\sim 10^{10}$  potential descriptors

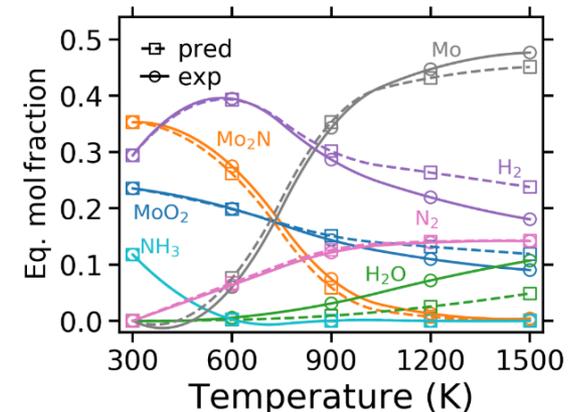


- **92% accurate** single descriptor identified to predict perovskite stability — significantly reducing # of DFT calculations
- **Enabling** high-throughput predictions of energetics and thermochemical equilibrium
- Collaboration with the **NREL node**

*Descriptor for perovskite stability*



*Simulated equilibrium using Gibbs energy minimization in virtual reactor*



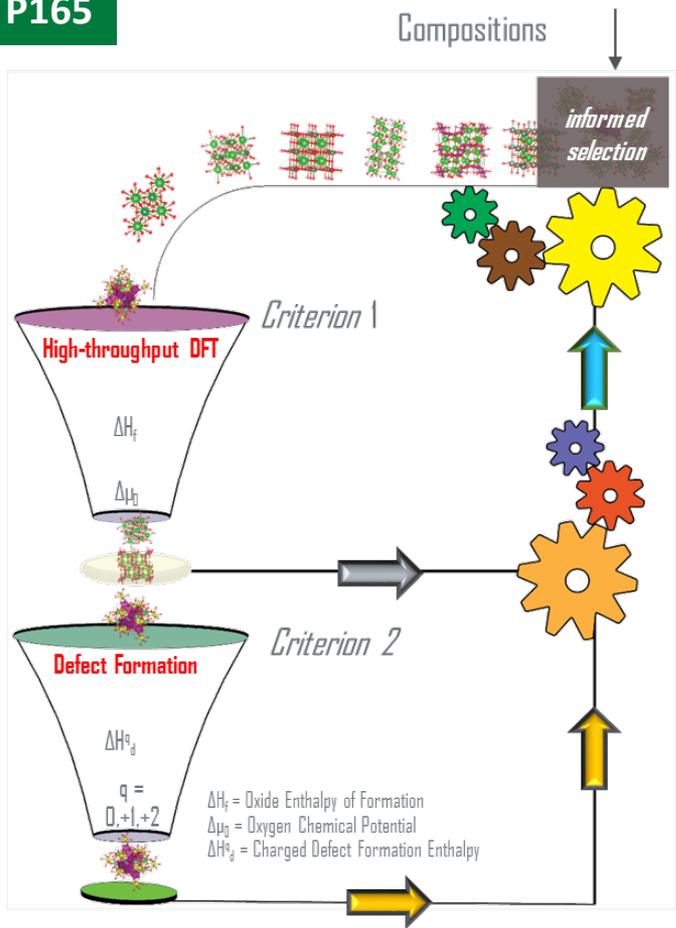
**Machine learning, high-throughput and combinatorial approaches enable accelerated STWS materials discovery**



# HydroGEN: Exciting Accomplishments

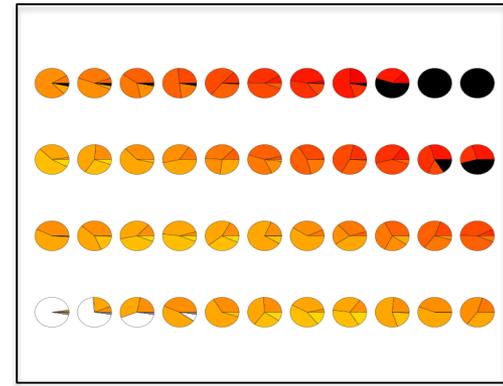
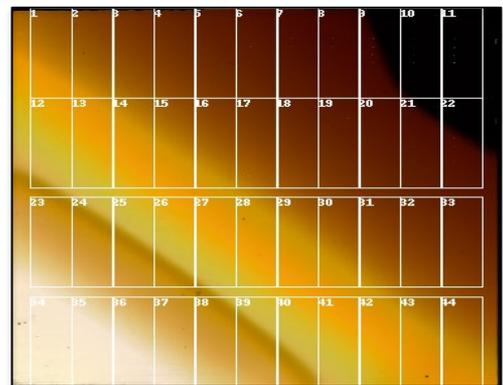
## Solar Thermochemical H<sub>2</sub> Production

P165



Colorado School of Mines has:

- Developed a **high-throughput** computational & **combinatorial** experimental approach to accelerate materials discovery
- Successfully differentiated **thermochemically active** from *merely* thermal reducible compositions with a **single color measurement**



**Machine learning, high-throughput and combinatorial approaches enabling accelerated STWS materials discovery**



# Hydrogen Fuel R&D Highlights

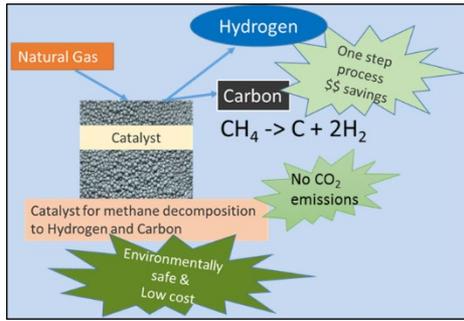
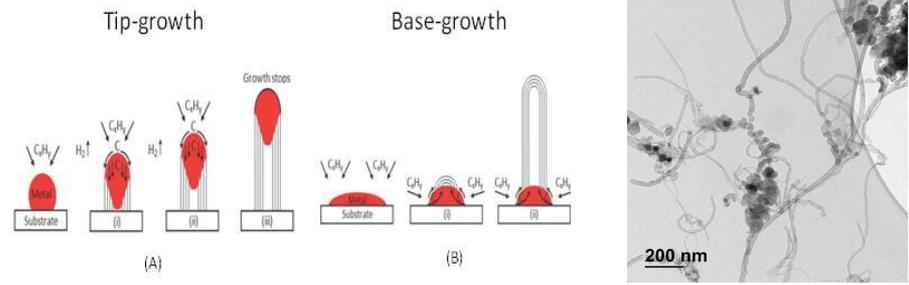
# Innovative Concepts

## Solid Carbon

IA019

Initiated projects with PNNL, NETL and University Coalition for Fossil Energy Research (UCFER) targeting production of low-cost base-growth carbon fibers through catalytic methane pyrolysis.

- **Objective:** Utilize cheap domestic Natural Gas to produce CO<sub>2</sub>-free H<sub>2</sub> and value added solid carbon materials.

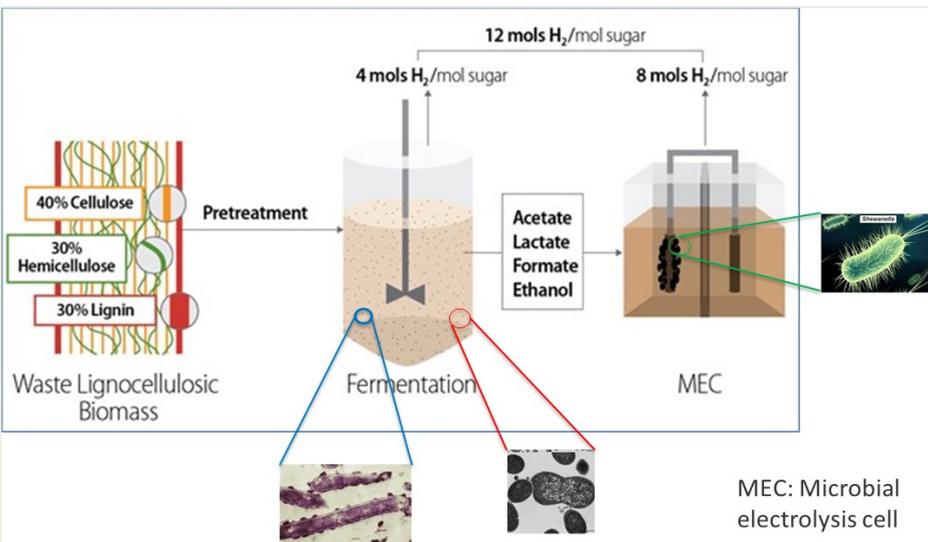


## Biological H<sub>2</sub>

P179

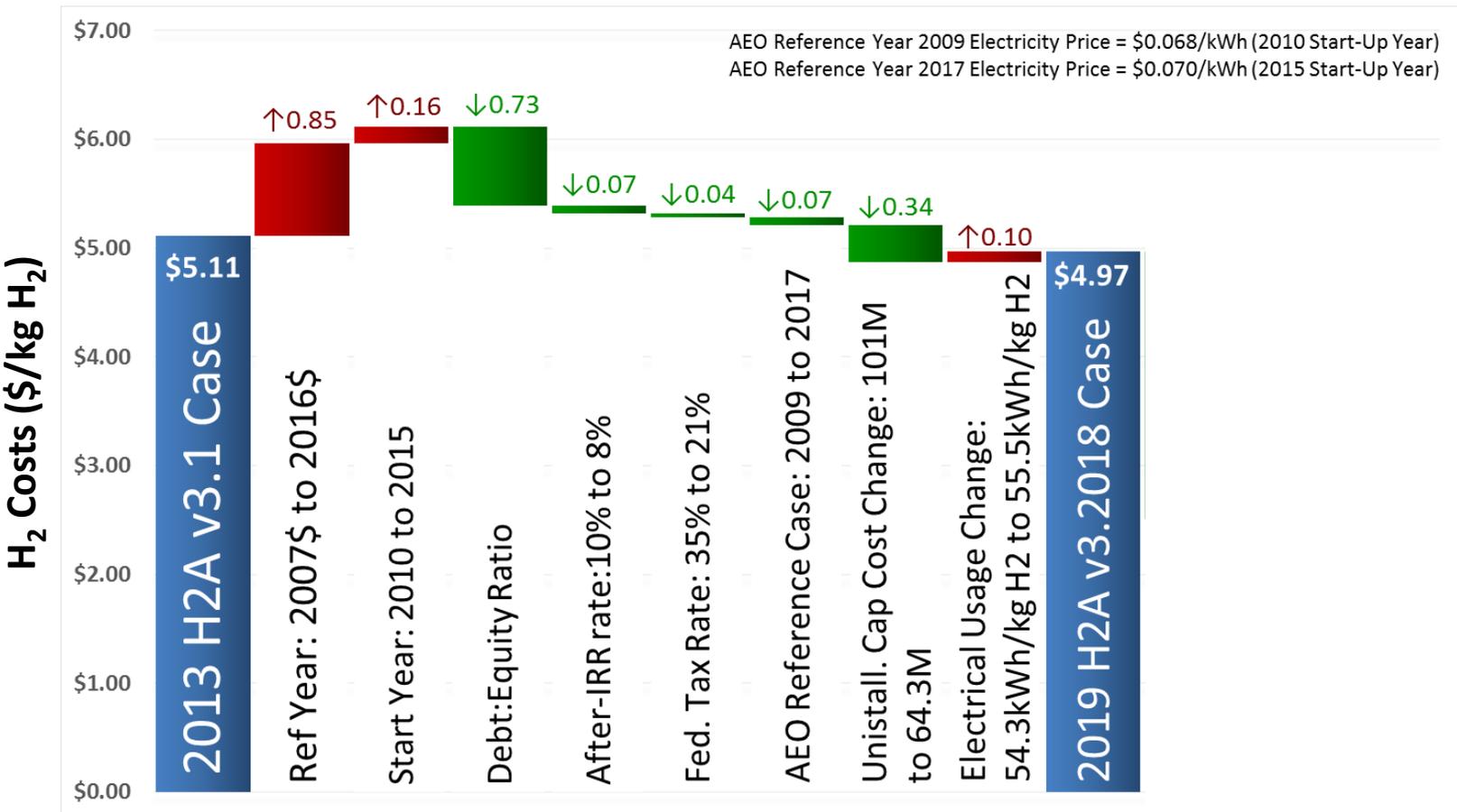
Initiated multi-Lab BioH<sub>2</sub> Consortium

- **High-solid loading** fermentation technology to convert renewable biomass resources into H<sub>2</sub>
- Integration with innovative microbial electrolysis cell (MEC) to **increase yield**



# Updated cost analysis for LTE H<sub>2</sub> production

## Current case – Preliminary results

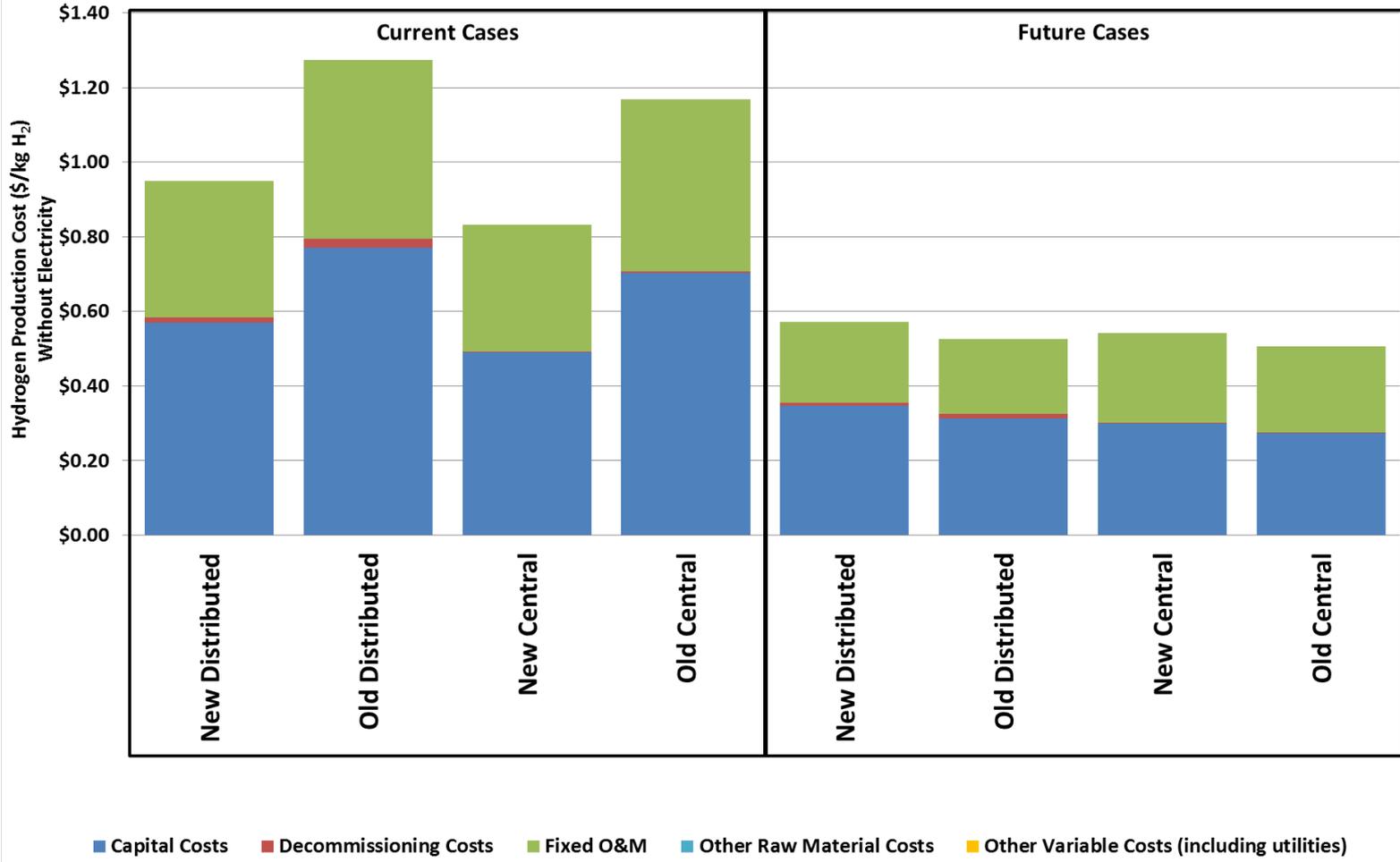


**Cost of H<sub>2</sub> production by low-temperature PEM electrolysis updated to reflect current assumptions and realities – net result – *slight reduction in cost***

# Updated PEM system costs in H2A

PEM H2A cost results (without electricity cost)

Preliminary results



Updated PEM cost analyses show reduced contribution from current system capital costs

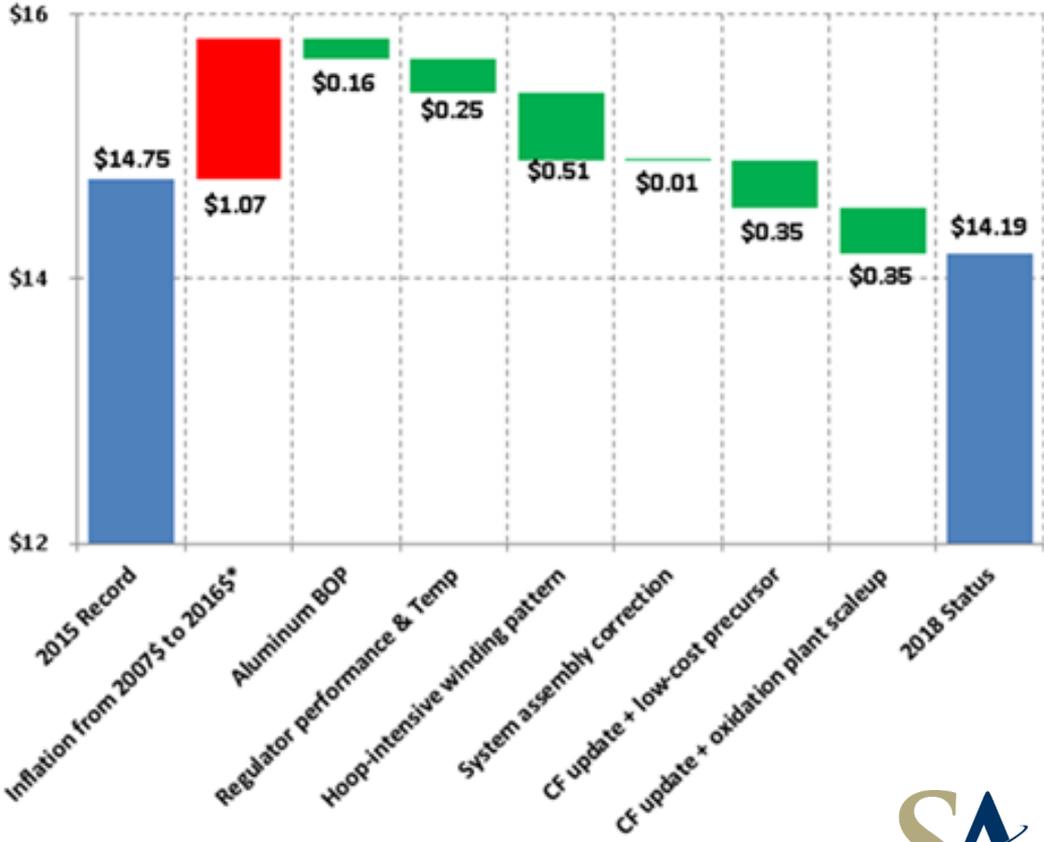
# Updated onboard storage cost record

Major changes from 2015 to 2018:

- Change from 2007\$ to 2016\$ basis (1.64% average annual rate of inflation)
- Change in Toray T700S carbon fiber baseline cost
- Improvement in performance of various components

Net result: cost reduction from \$14.75 to \$14.19 per kWh (4% reduction) at 500k systems per year

*Note: volume projections are being revised from 500k systems per year, to 100k systems per year*



Improvements are continuously driving down costs, however costs are dominated by carbon fiber costs

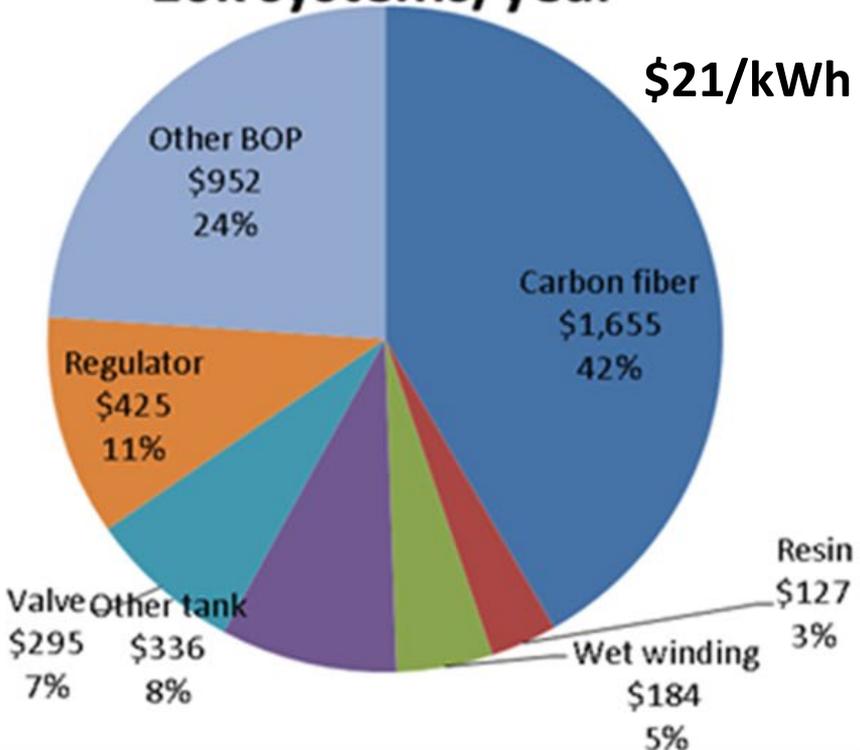
# System cost breakdown

Carbon fiber costs dominates cost of 700 bar COPV systems, however significant cost reductions still can be made in BOP components

ST100

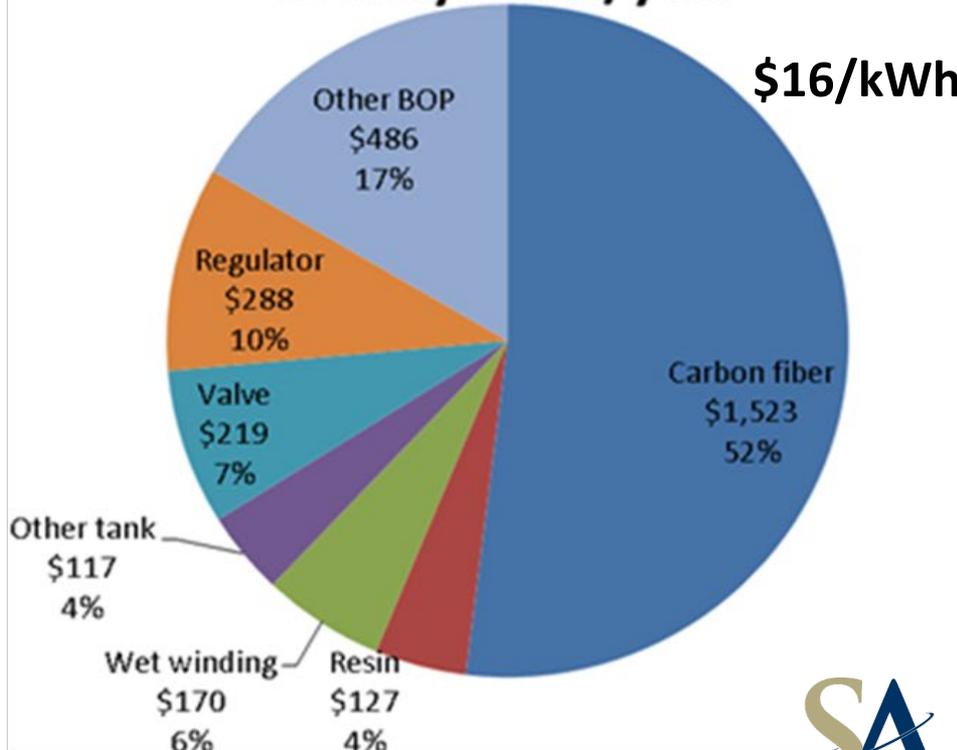
10k systems/year

\$21/kWh



100k systems/year

\$16/kWh

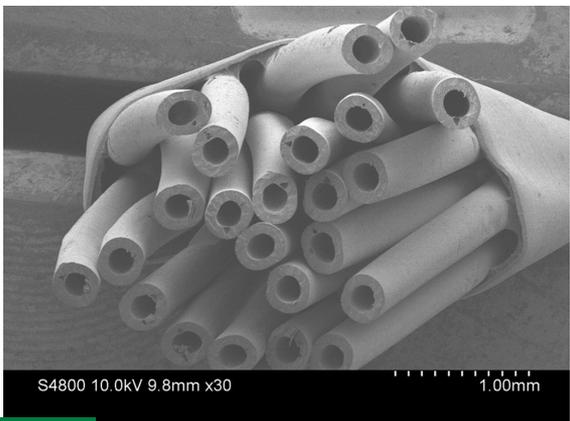


Single tank, 700 bar COPV onboard systems with 5.6 kg H<sub>2</sub> usable capacity

# Reducing Carbon Fiber Cost through Precursors

## Improved processing and development of hollow PAN precursor fibers

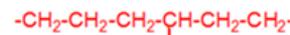
- 50% reduction in wastewater = 5% reduction in carbon fiber cost
- Spun hollow PAN fibers without bore fluid



ST146

## Development of low-cost polyolefin precursor fibers with high mass yield

PE-co-Pitch precursor

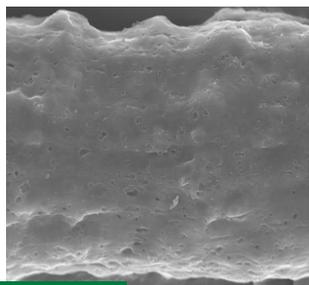


+

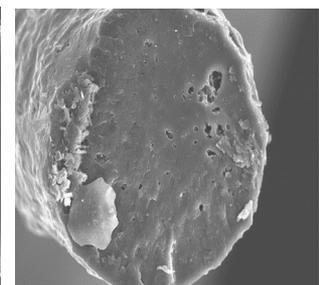


Some unattached Pitch serving as Plasticizer

> 70% mass yield demonstrated on carbonization

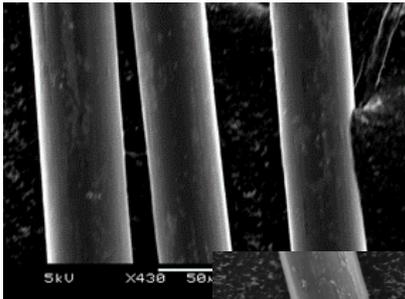


ST147

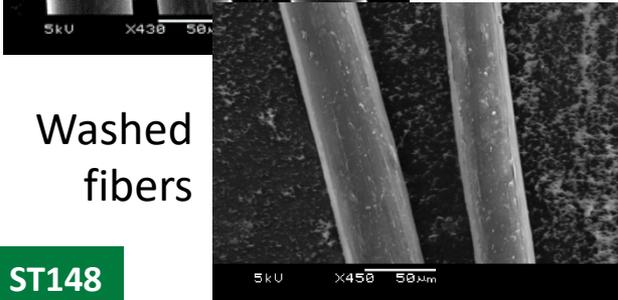


## Novel plasticized PAN fibers produced through low-cost melt spinning

Ionic liquid	PAN (%)	As Spun Diameters (μm)	Washed Fiber Diameters (μm)
[C <sub>3</sub> mim]Br	30	56.2 +/- 0.16	53.4 ± 7.6
[C <sub>4</sub> mim]Br	30	56.8 +/- 0.20	45.6 ± 7.9
[C <sub>4</sub> mim]Cl	30	54.7 +/- 0.08	45.3 ± 8.7
[MPCNIm]Br	30	59.6 +/- 0.25	47.9 ± 14.1
[MPCNIm]Cl	30	53.4 +/- 0.17	48.6 ± 10.4



As spun fibers



Washed fibers

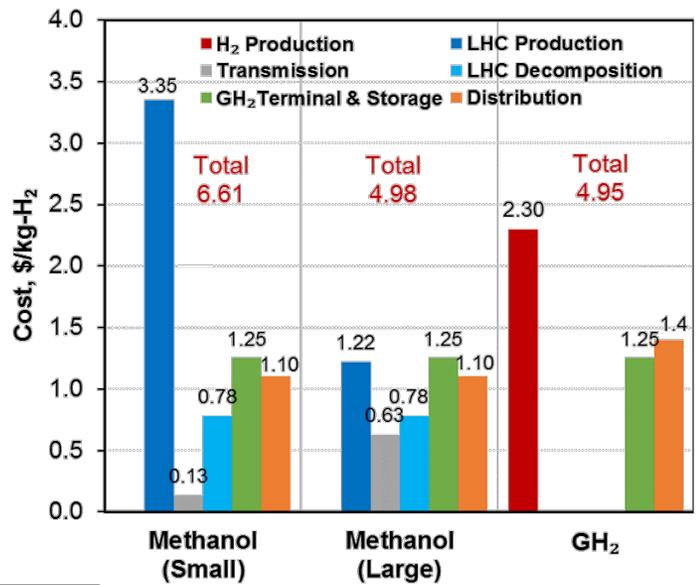
ST148

*PAN precursor fibers represent approximately 50% of the cost of carbon fiber, with the other 50% coming from the conversion processing*

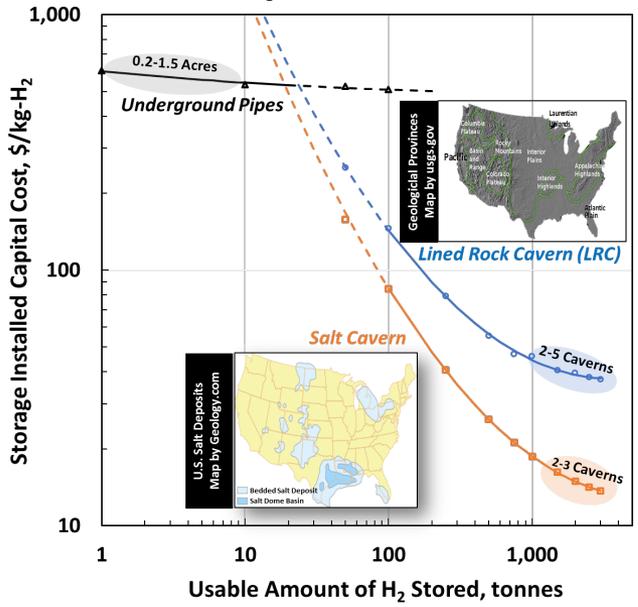
# Technologies for transport and bulk storage

## Techno-economic analysis to determine baseline for Hydrogen Carriers and Bulk Hydrogen Storage

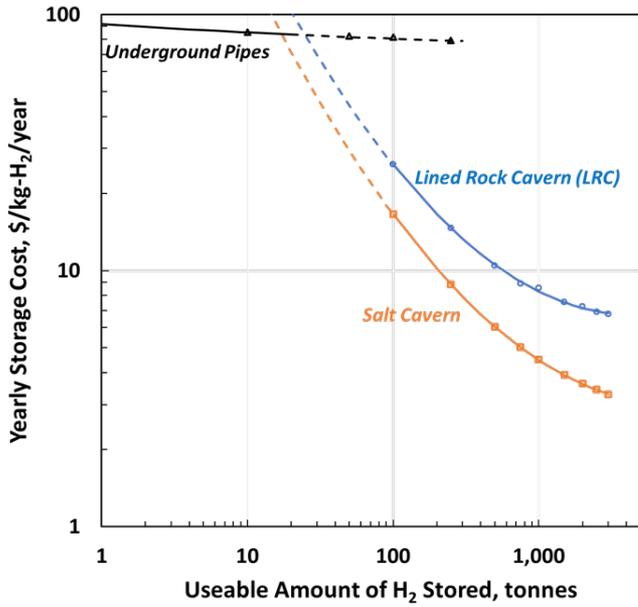
- 50 tonne per day H<sub>2</sub> usage
  - MCH, NH<sub>3</sub>, and MeOH base cases
  - MeOH competitive with compressed H<sub>2</sub> even when transported 3000 km from gulf coast
- 500 tonne (10 day) bulk storage
  - Underground pipe, lined rock caverns and salt dome geologic storage base cases



### Capital costs



### Annual costs



**Preliminary results, geologic storage can be 1/10<sup>th</sup> the costs of underground compressed gas at high capacities, but underground compressed is more cost effective up to ~20 tonne capacities**

# Hydrogen Interface Taskforce (H<sub>2</sub>IT)

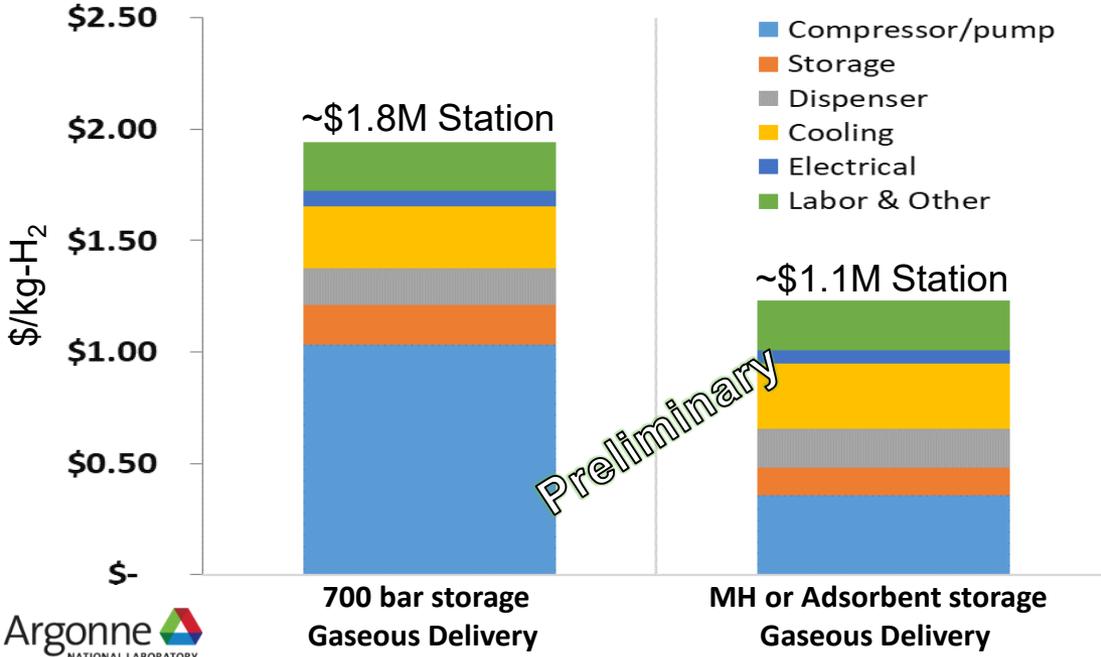


Cross TT taskforce developing a holistic H<sub>2</sub> pathway analysis across emerging H<sub>2</sub> production, delivery & onboard storage technologies

Storage System	Operating Temperature	Operating Pressure
700 bar Compressed H <sub>2</sub>	Ambient (-40 to 85°C)	5 bar to 875 bar
Metal hydride (MH) or Adsorbent	Near ambient to 120°C	5 to 100 bar

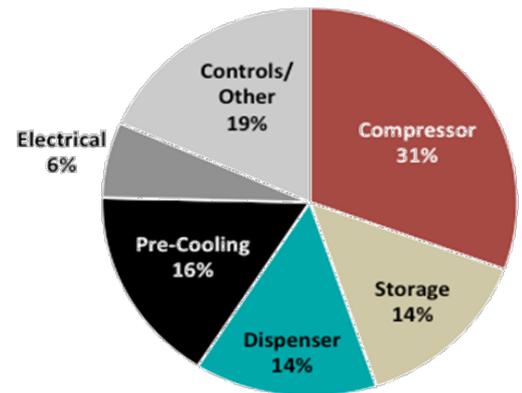
- Assumptions:
- Sacramento, 50,000 FCEVs (~2030), [2016\$]
  - 37 HRS (1000 kg/day capacity)
  - Manufacturing volume/learning
  - Truck delivery (500 bar)

## Contributions to H<sub>2</sub> Refueling Cost



- ~40% H<sub>2</sub> cost reduction
- ~40% station cost reduction
- Reduces burden at station (less compression / precooling)
- Improved station reliability

70 MPa station cost distribution



SA170

**Low-pressure, materials-based onboard storage enables lower H<sub>2</sub> & station costs**

# High-Impact Collaborative Initiatives

## Interagency Collaborations



### Collaborations between NSF projects and FCTO EMN consortia

- NSF-DMREF / HydroGEN EMN
- NSF-SSMC / HyMARC EMN



### Collaborations between DOD and FCTO H<sub>2</sub> Fuel R&D

- Navy - NUWC – materials-based storage for H<sub>2</sub>-FC UUV applications
- Army – DEVCOM C5ISR – developing alane (AlH<sub>3</sub>) production capacity
- Army – CCDC GVSC – onboard H<sub>2</sub> storage for combat vehicles



### Collaborations between DOC projects and FCTO EMN consortia

- NIST Center for Neutron Research / HyMARC EMN

## Interagency Collaborations



U.S. DEPARTMENT OF ENERGY

- Office of Science
- Office of Fossil Energy
- Office of Nuclear Energy
- Energy Efficiency & Renewable Energy

### Collaborations between FCTO H<sub>2</sub> Fuel R&D and:

- OS-BES, ARPA-E and EERE-SETO on solar fuels
- Fossil Energy and NETL on co-production of value-added products
- Nuclear Energy on high-temperature electrolysis
- EERE-BETO on synthetic fuels and biomass conversion
- OS-BES/BER on user facilities for EMN activities



# H<sub>2</sub> Fuel R&D presentations

- **Hydrogen Production:**
  - Tuesday, Regency Ballroom F, 8:30 am – 6:15 pm
  - Wednesday, Regency Ballroom E, 8:30 am – 10:00 am
    - Note the change in room between Tuesday and Wednesday
- **Hydrogen Storage**
  - Wednesday, Regency Ballroom F, 8:30 am – 5:45 pm
- **H<sub>2</sub> Fuel R&D Posters**
  - Tuesday, Independence Center A&B, 6:30 - 8:00 pm

# Thank you from the Hydrogen Fuel R&D Team

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