U.S. DEPARTMENT OF
ENERGY

Office of
ENERGY EFFICIENCY &
RENEWABLE ENERGY

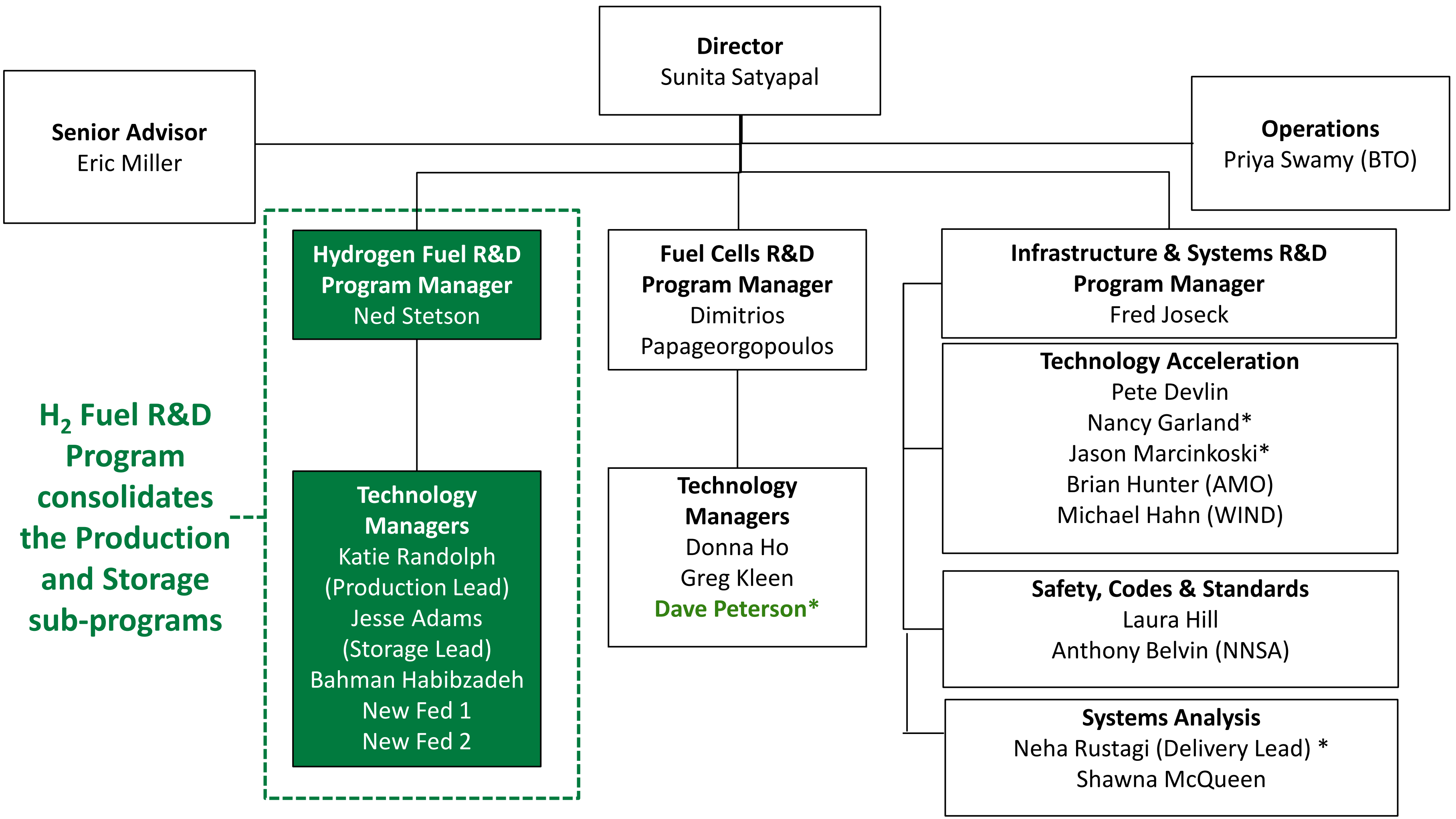
H_2 Fuel R&D Overview

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_2 production

Hydrogen Storage

Research and Development

- Low-cost storage technologies
- High-capacity materials-based storage technologies
- Cost effective transport bulk storage and technologies, enabling H2@Scale

Ultimate Goal

Less than $8/kWh

for onboard storage

Collaboration through Consortia

HyMARC — Enabling twice the energy density for onboard H_2 storage

H-Mat Hydrogen Materials Compatibility Consortium — 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

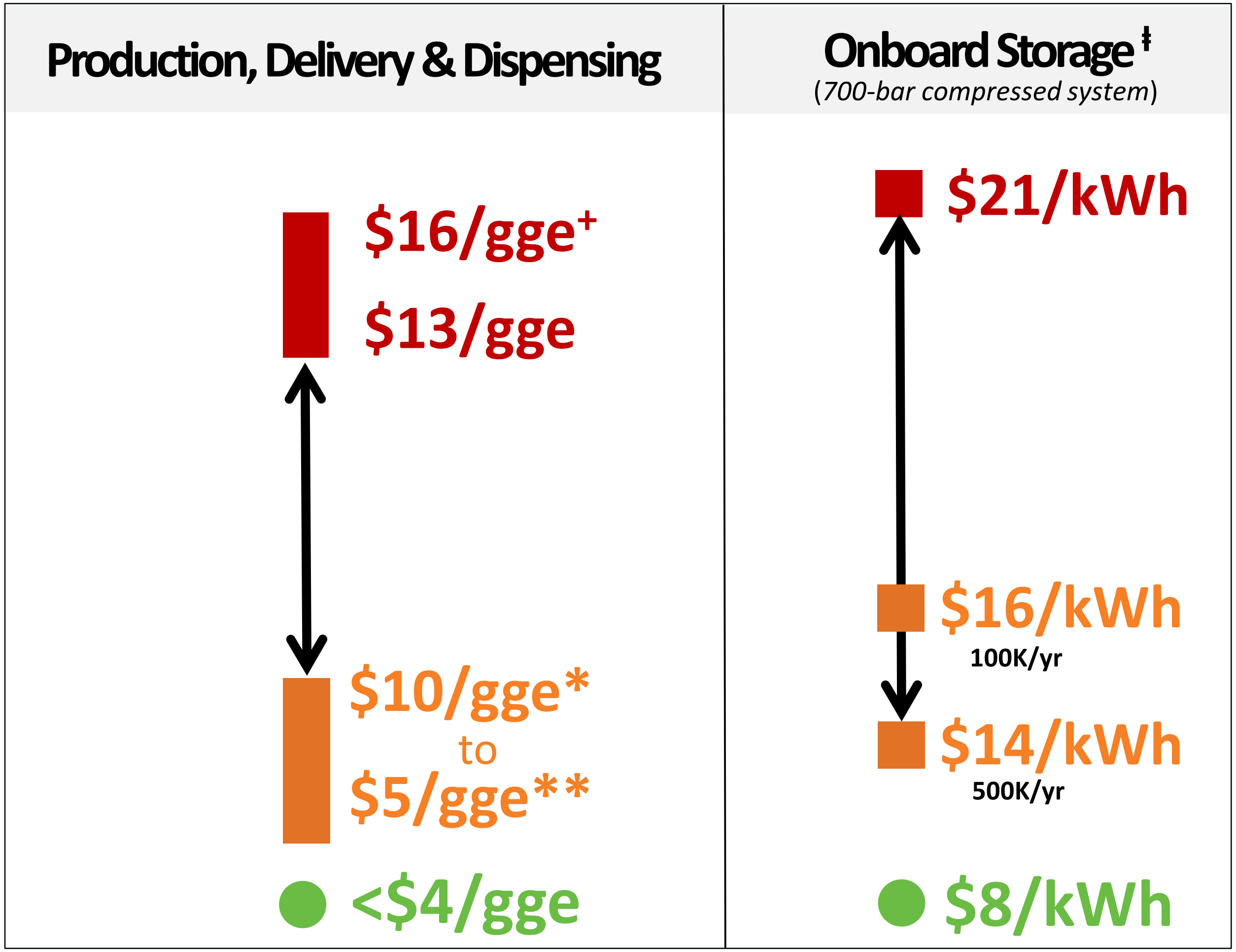
Storage

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_2 Fuel Portfolio helps enable

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

Cost Targets and Status

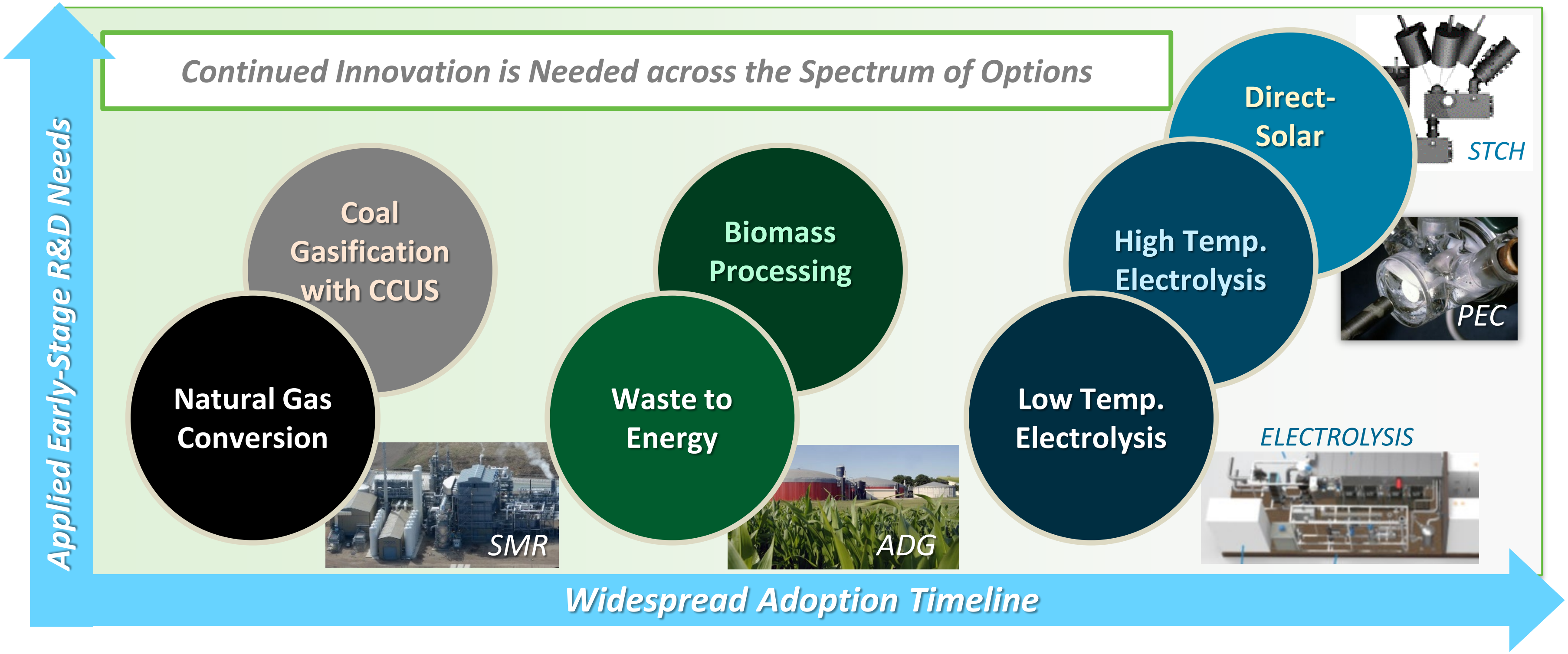


† Range assumes current production from NG and delivery and dispensing
* Highest possible cost at high vol., assumes H2 from electrolysis at $5/gge and delivery via pipelines and liquid tankers at $5/gge
** Lowest possible cost at high vol., assumes H2 from SMR at $2/gge and delivery via tube trailer at $3/gge
ǂ 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_2 Production R&D



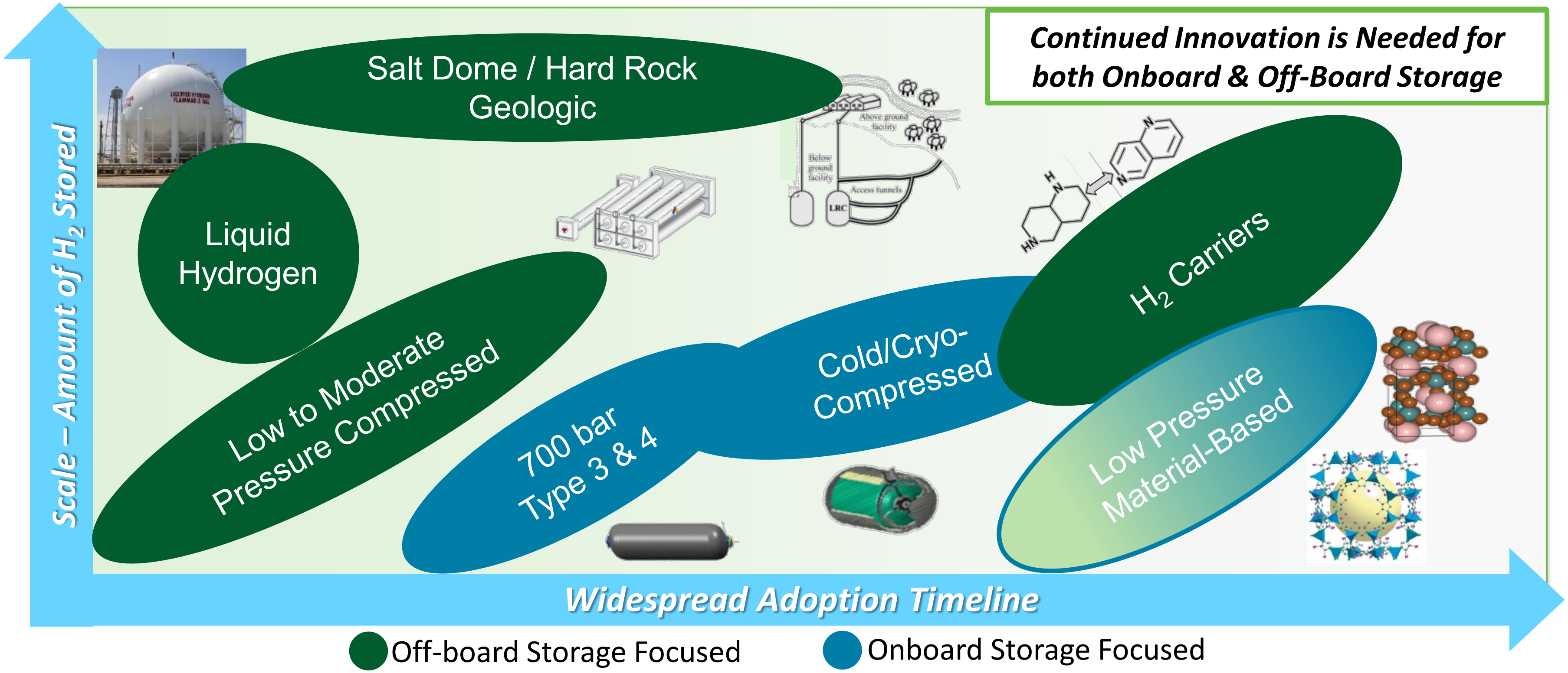
Innovative Concepts: Fossil Fuels/Waste/Biomass

- 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_2 Storage R&D



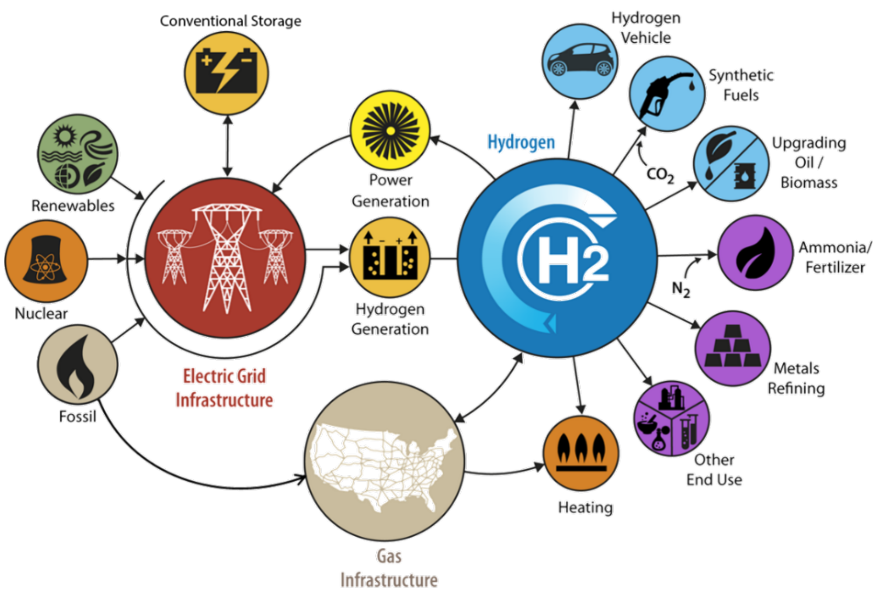
Off-Board Focus Areas

- H_2 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_2 Fuel R&D Topics



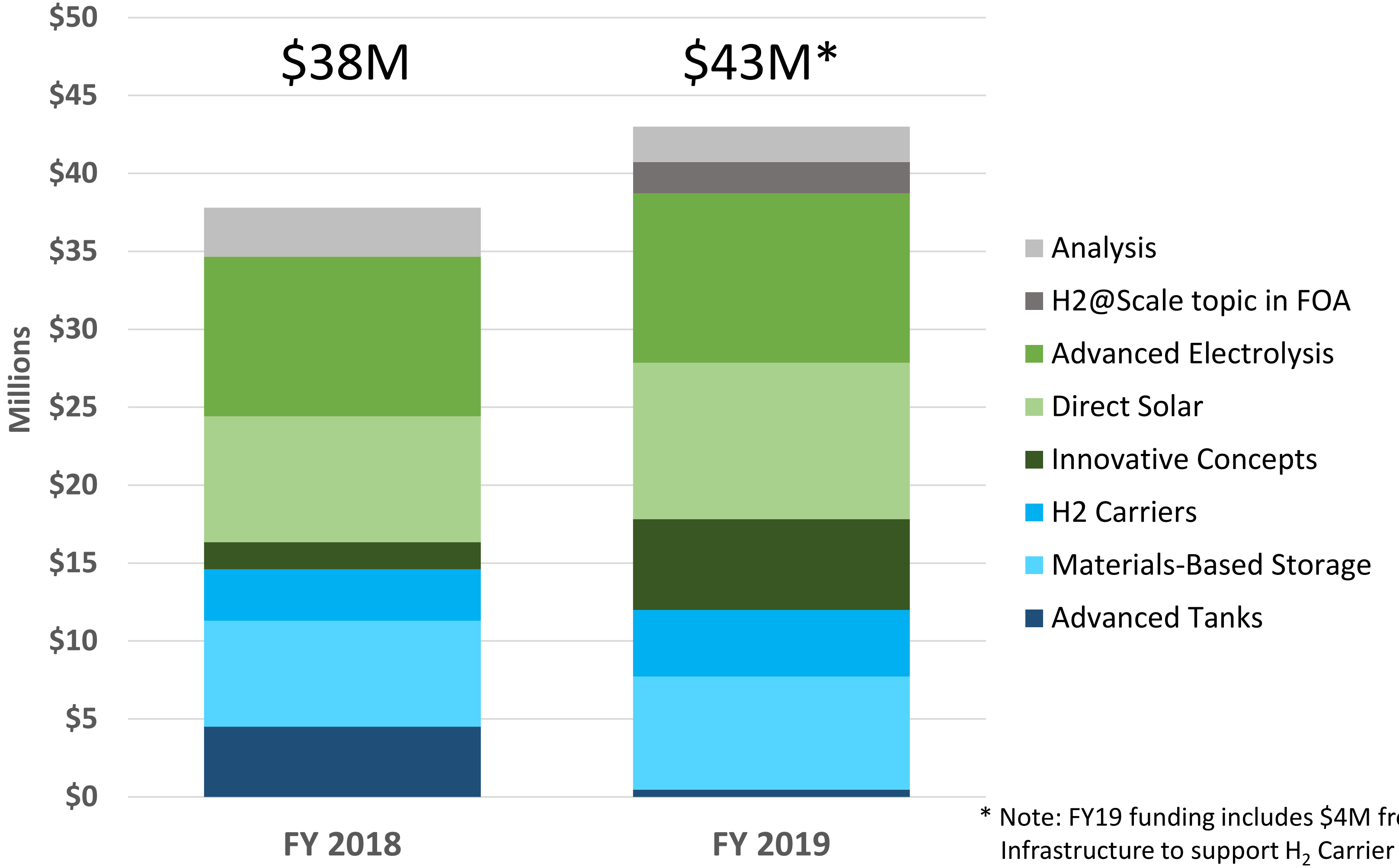
FY 2019 H2@Scale FOA

- Total funding up to $31M
- Early stage R&D topics in storage and production include:
  - **Advanced H_2 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



* Note: FY19 funding includes $4M from Infrastructure to support H_2 Carrier R&D

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

H_2 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_2 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_2 Fuel R&D, and Safety, Codes, and Standards

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

Dispensing Hoses

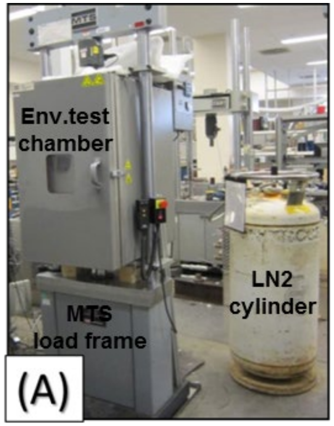
Hydrogen Storage

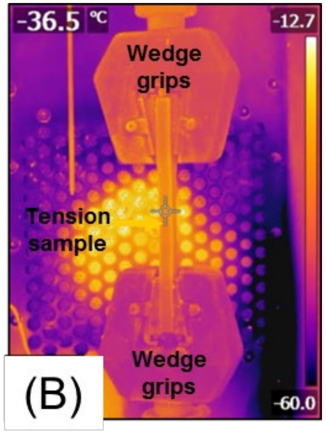
Hydrogen Pipelines

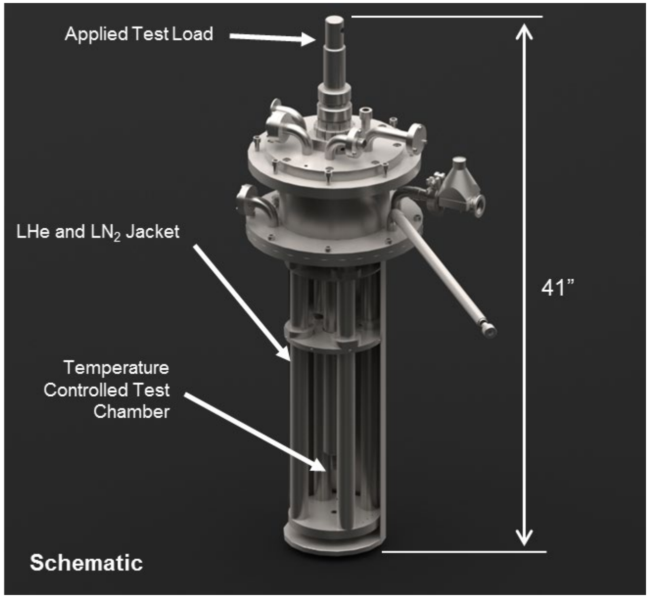
IN001 & SCS026

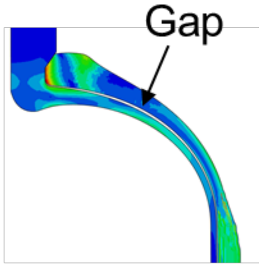
H-Mat: Understanding impact of cryogenic operation on materials

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









CF/Epoxy and aluminum liner after cooling down (80K)

Computational analysis to guide experimental research

Pacific Northwest NATIONAL LABORATORY

Sandia National Laboratories

OAK RIDGE National Laboratory

Argonne NATIONAL LABORATORY

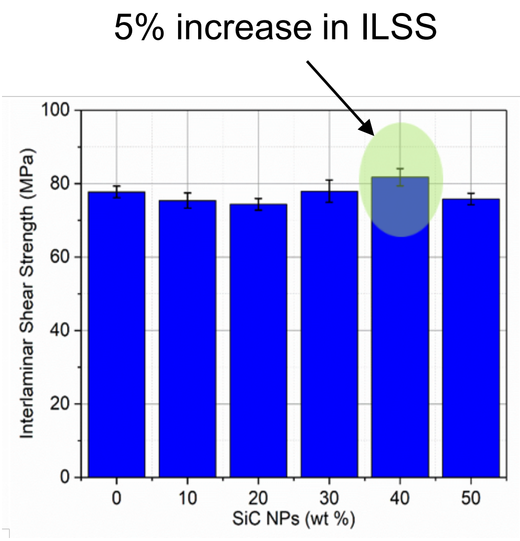
ST200

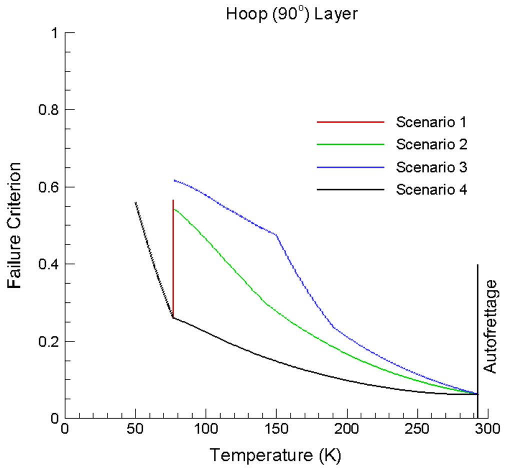
There is a need to understand the impact of thermal and pressure cycling on the performance of materials used within the hydrogen infrastructure

H-Mat℠ Hydrogen Materials Compatibility Consortium

H-Mat: Accomplishment Summary

- Thermomechanical techniques for temperatures down to -140˚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





ST200

HyMARC

HyMARC: Accelerating the development of viable hydrogen storage materials

Enabling twice the energy density for hydrogen storage

Individual Seedling Projects

National Lab Team

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

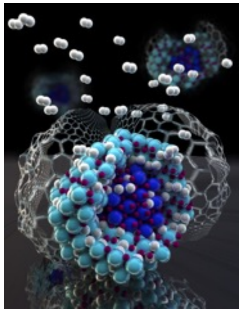
Seedling Projects

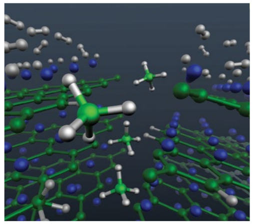
- Applied material development
  - Novel material concepts
  - High-risk, high-reward
- Concept feasibility demonstration
- Advanced development of viable concepts

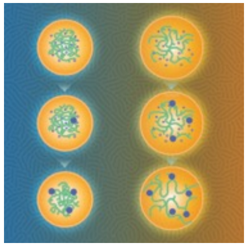
HyMARC Phase II successfully kicked-off, two separate lab teams fully integrated together into the HyMARC effort

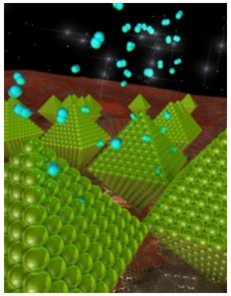
HyMARC: Disseminating Phase 1 results

- > 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	Task 2	Task 3	Task 4	Task 5	Task 6
Sorbents	**Hydrides**	**Carriers**	**Adv. Char.**	**Seedling Support**	**Data Hub**
Gennett	Allendorf	Autrey	Parilla (NREL validation) Prendergast (ALS, SLAC, MF) Bowden (PNNL NMR) Brown (NIST Neutron) Toney (SLAC, X-ray)	Allendorf Gennett	Munch (NREL)
Focus Areas	**Focus Areas**	**Focus Areas**	**Focus Areas**		

Task leads:
Coordinate work
Milestone accounting
Reporting

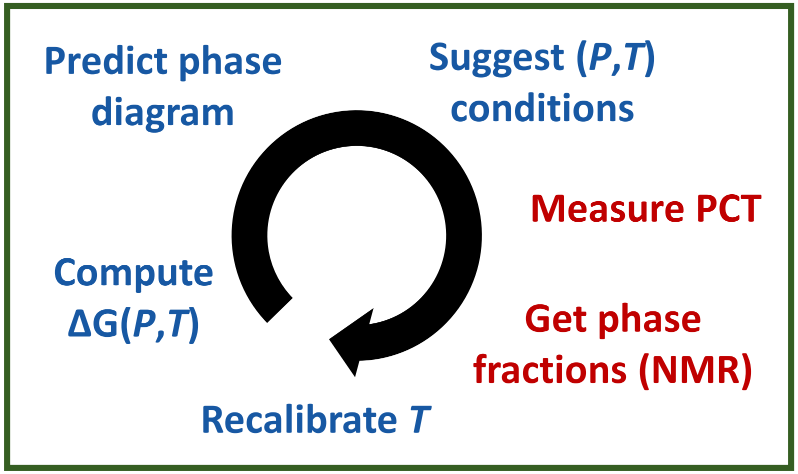
Focus Areas (new concept):
Multi—lab Research clusters
Defined topic
Dynamic, agile
Duration: as little as 1 year
Applied topics: Go/No-Go
Foundational topics: milestones

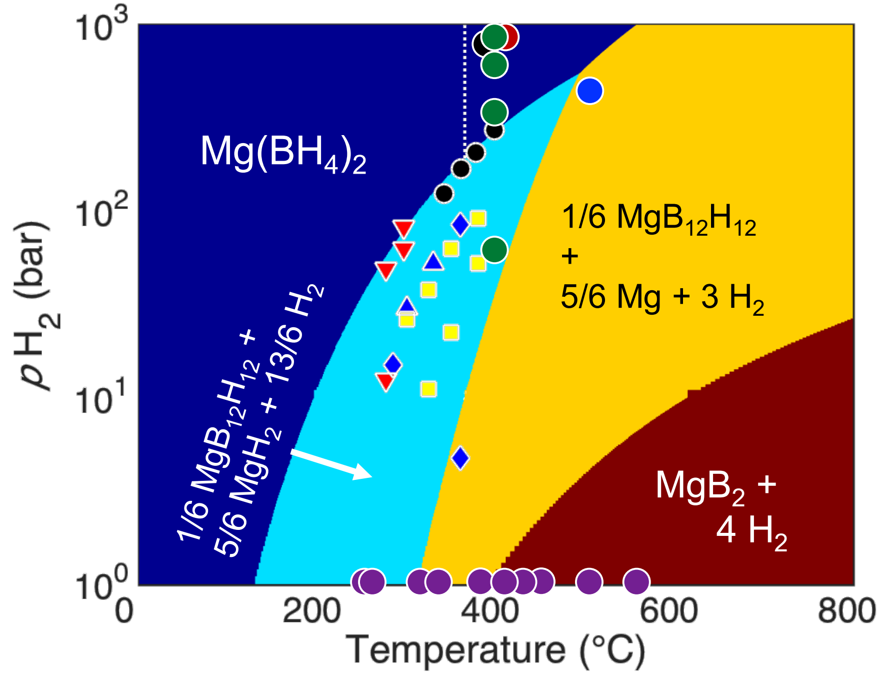
User Facility POCs

ALS, SLAC, NREL, NIST, EMSL, MOLECULAR FOUNDRY

ST127

HyMARC: Close coupling of computation and experiment





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

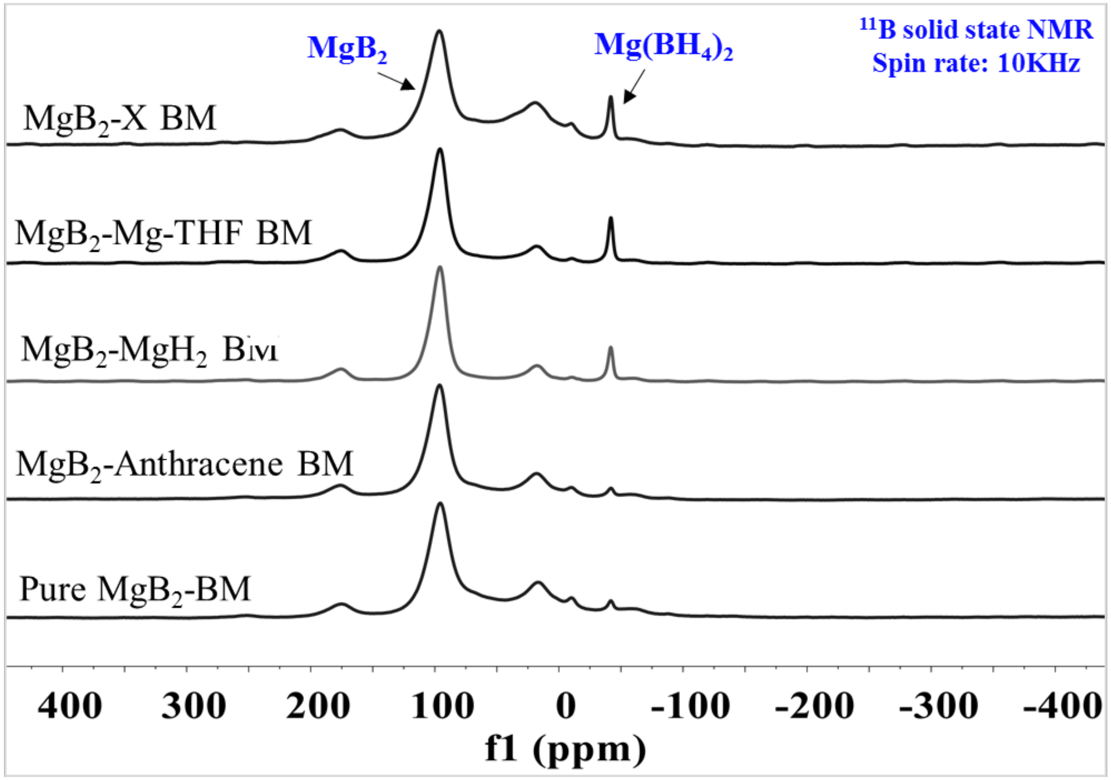
ST129

Example: Accurate bulk phase diagram prediction and validation

HyMARC: Exciting new preliminary results

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

$$MgB_2\text{–}10\ \text{mol\%}\ X + H_2 \xrightarrow[<250\ ^oC]{<200\ \text{bar}} Mg(BH_4)_2$$



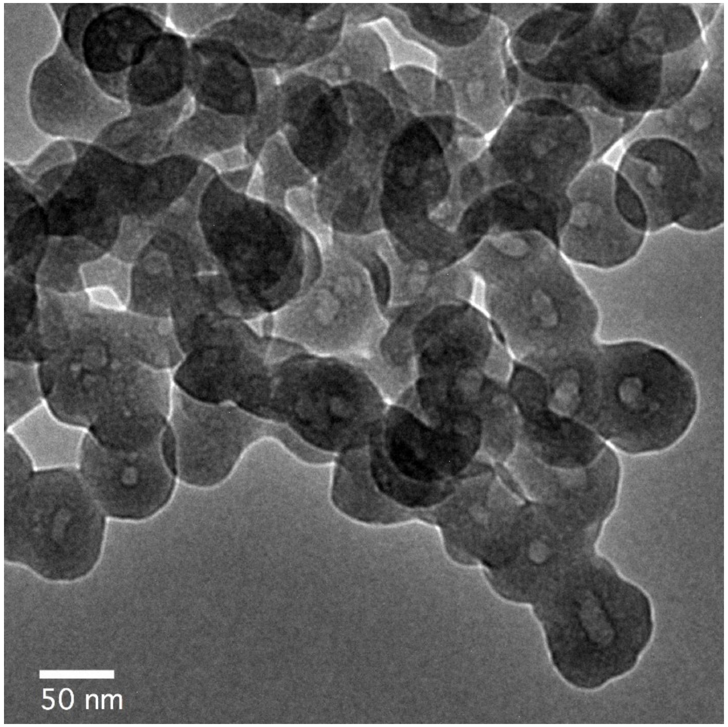
Demonstrated formation of $Mg(BH_4)_2$ under conditions of ***less than 200 bar and 250 °C***, significantly reduced from prior 700 bar and 300 °C required conditions.

ST138

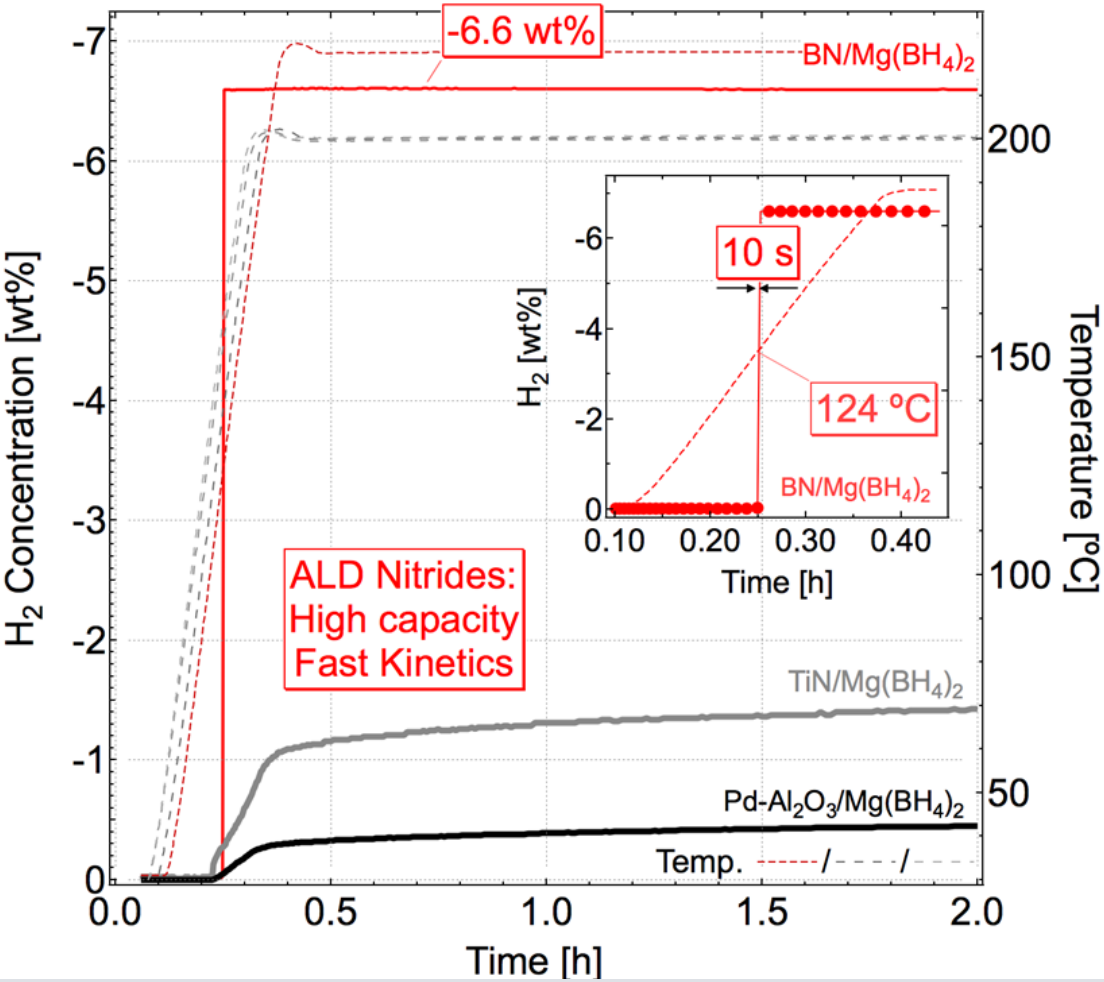
Additives are effective in reducing required hydrogenation conditions for MgB_2

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

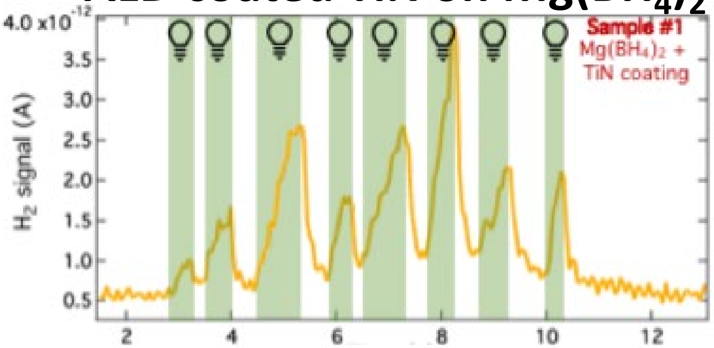
NREL NATIONAL RENEWABLE ENERGY LABORATORY

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

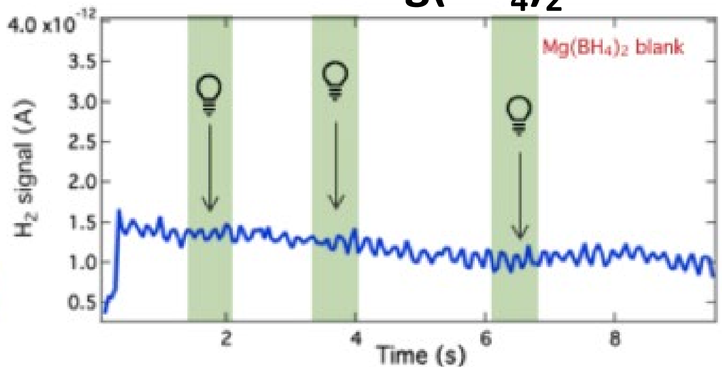
HyMARC: Exciting new preliminary results

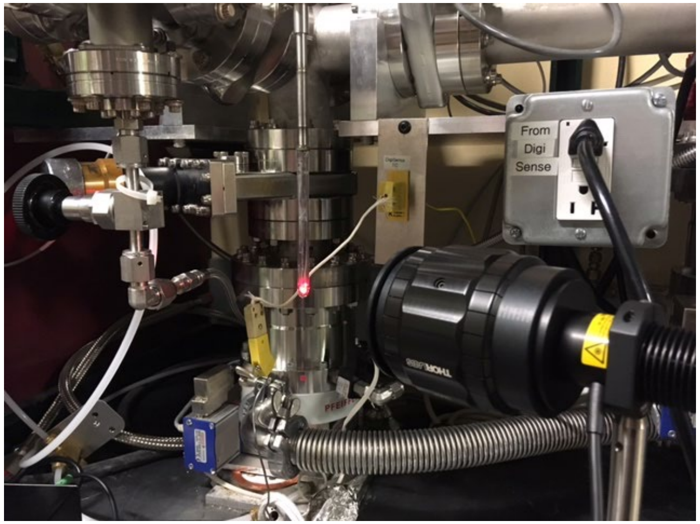
Controlled hydrogen release from $Mg(BH_4)_2$ using light! (NREL)

ALD coated TiN on $Mg(BH_4)_2$

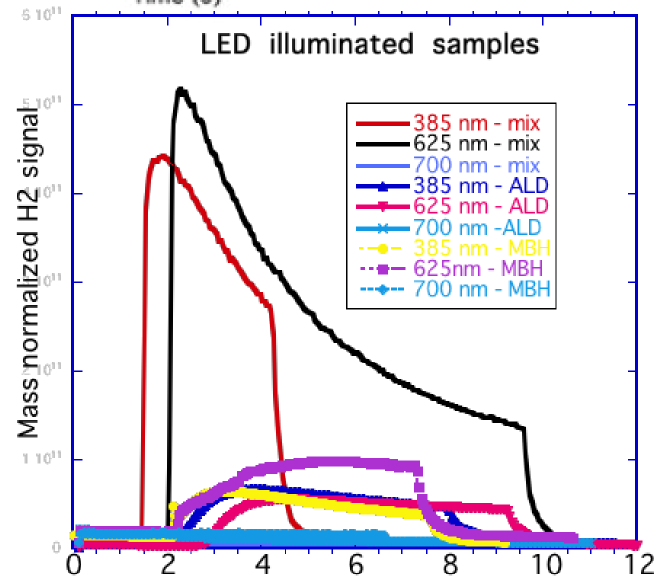


$Mg(BH_4)_2$





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



ST131

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

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

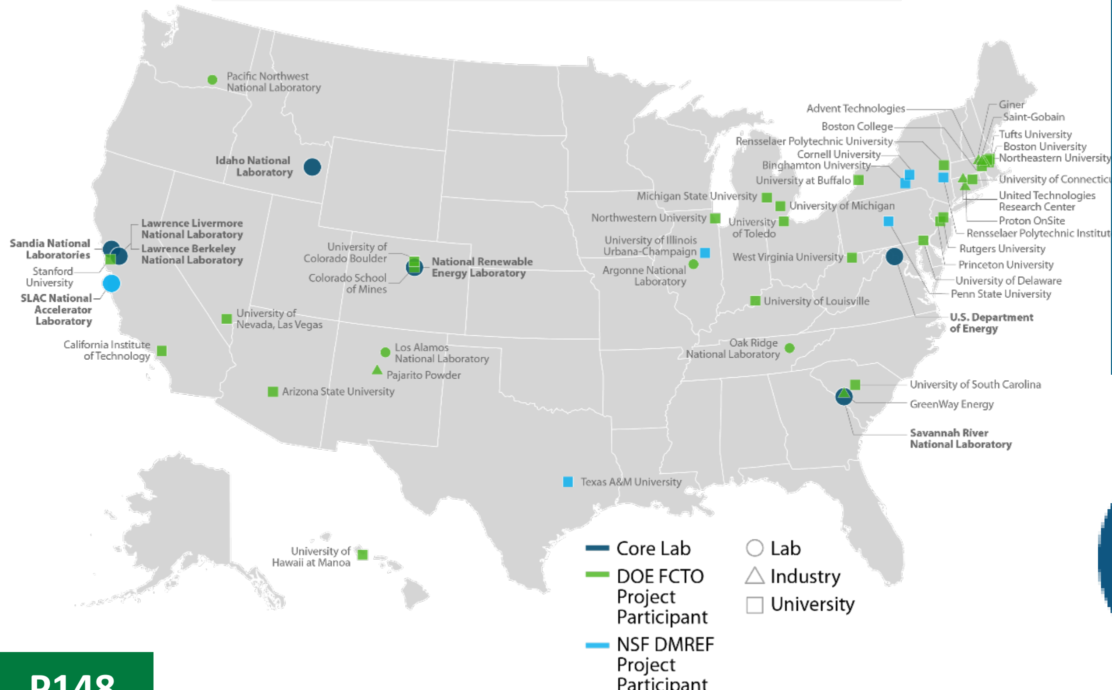
HydroGEN

Pioneering Research in Water Splitting

HydroGEN
Advanced Water Splitting Materials

NREL · Berkeley Lab · Sandia National Laboratories · INL Idaho National Laboratory · Lawrence Livermore National Laboratory · SRNL

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 $Ba_4CeMn_3O_{12}$ & 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

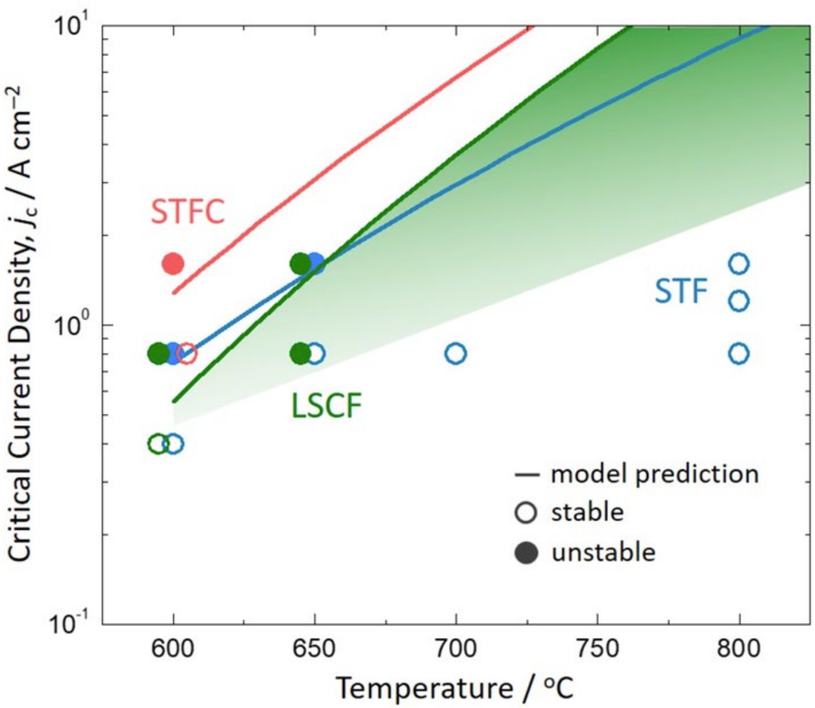
***LTE/PEC*: Multiscale, Multi-Theory Modeling to Understand the Oxygen Evolution Reaction Across pH Ranges**
Led LLNL and LBNL with NREL—integrating 6 nodes

HydroGEN: Exciting Accomplishments

High Temperature Electrolysis

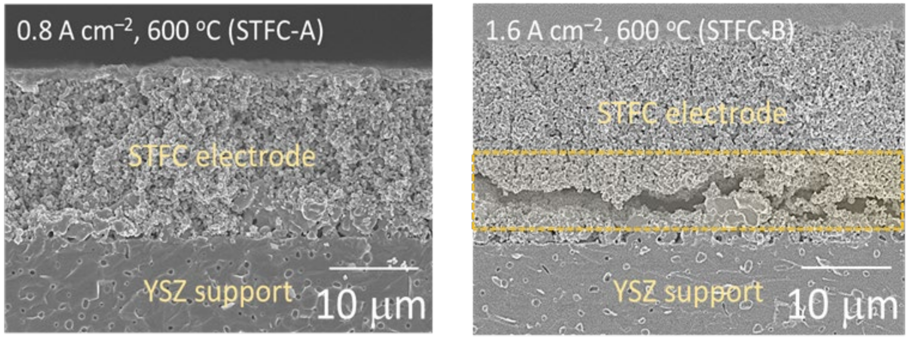
P153

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

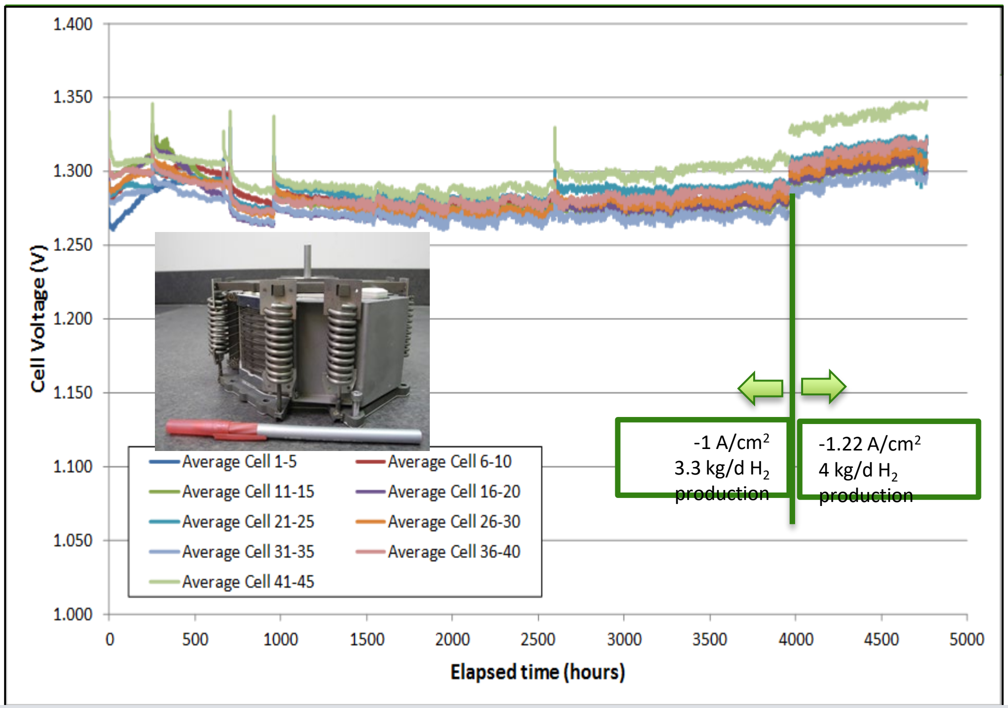
H_2 Production: Exciting Accomplishments

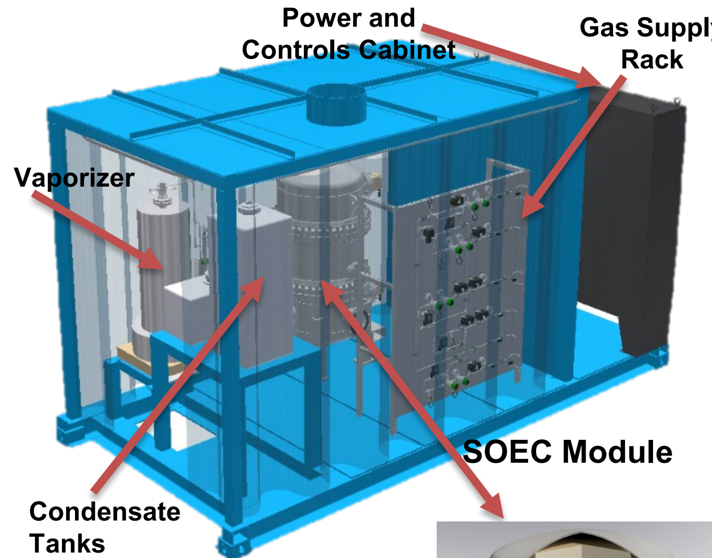
High Temperature Electrolysis

TA019

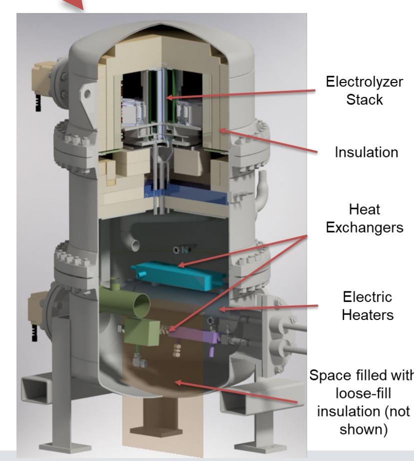
FuelCell Energy

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





>4 kg H_2/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

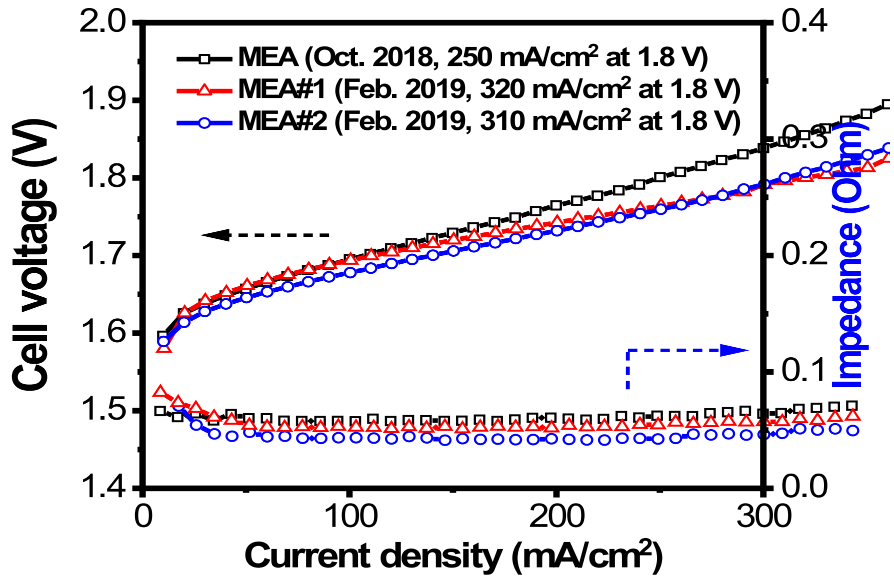
HydroGEN: Exciting Accomplishments

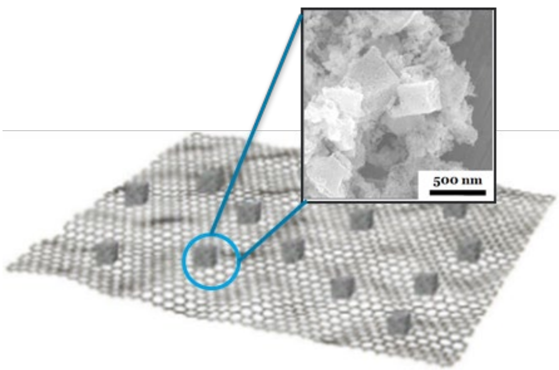
Low Temperature Electrolysis

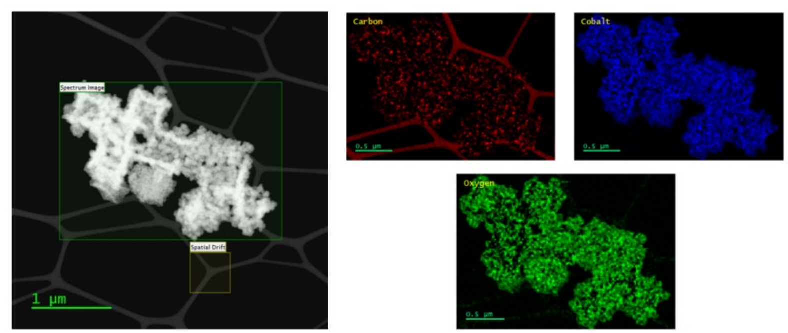
P157

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 mA/cm^2 at 1.8 V (testing at Giner)







Argonne NATIONAL LABORATORY

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

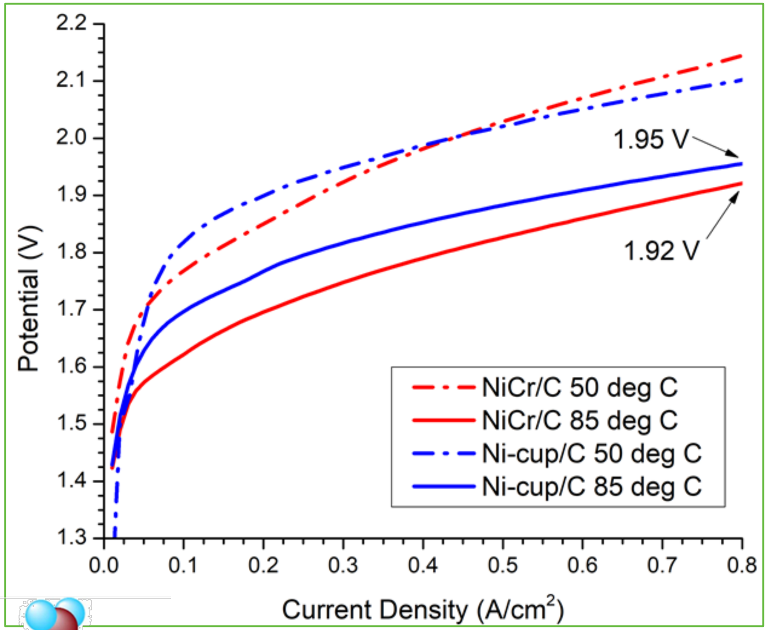
HydroGEN: Exciting Accomplishments

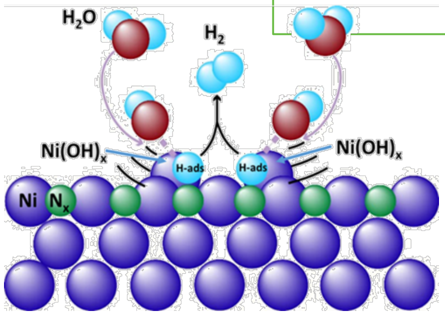
Low Temperature Electrolysis

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^2 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

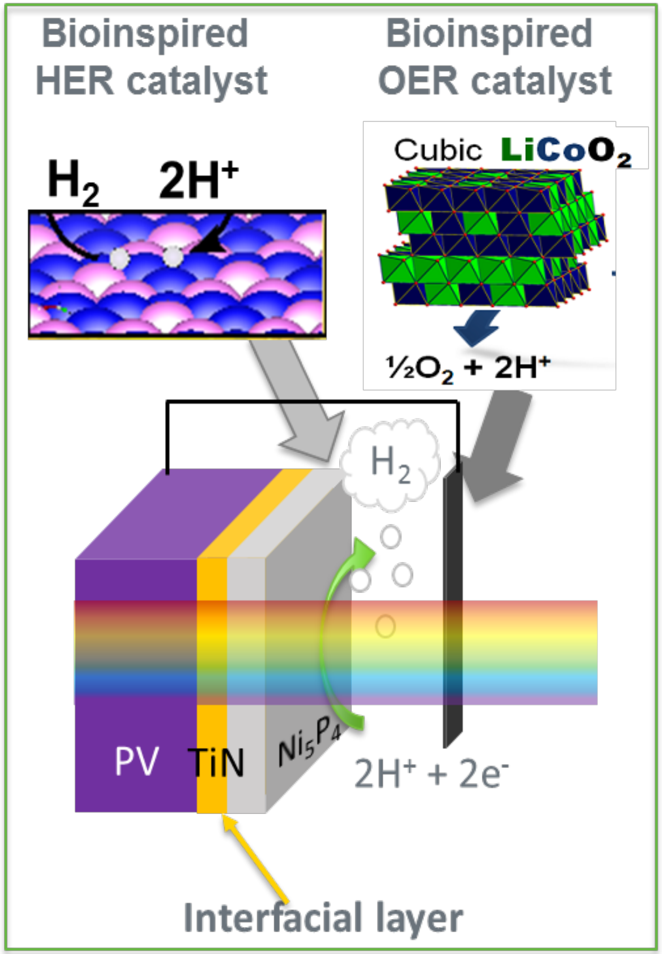
Photoelectrochemical H_2 Production

P160

RUTGERS 250 1766-2016

Rutgers demonstrated a:

- **Bioinspired** high solar-to-hydrogen efficiency system
- **11.5% with PGM-free** Ni_5P_4 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!

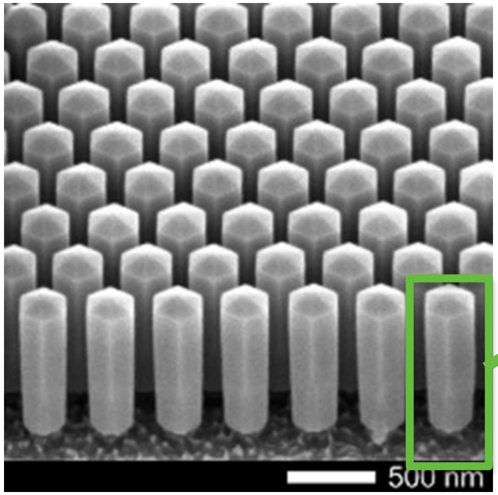
HydroGEN: Exciting Accomplishments

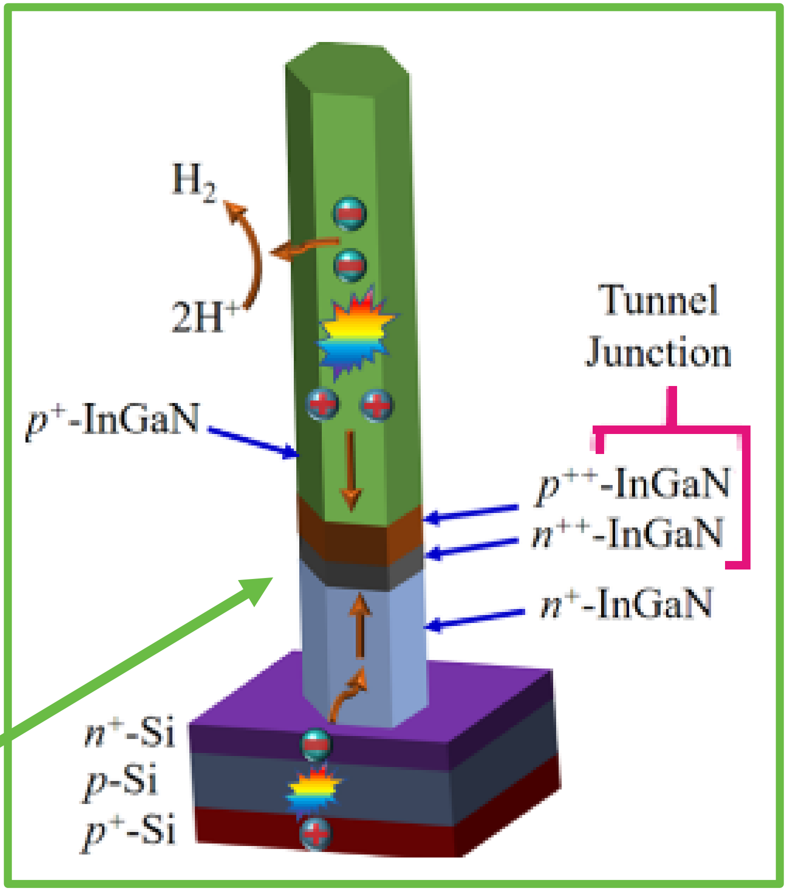
Photoelectrochemical H_2 Production

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!

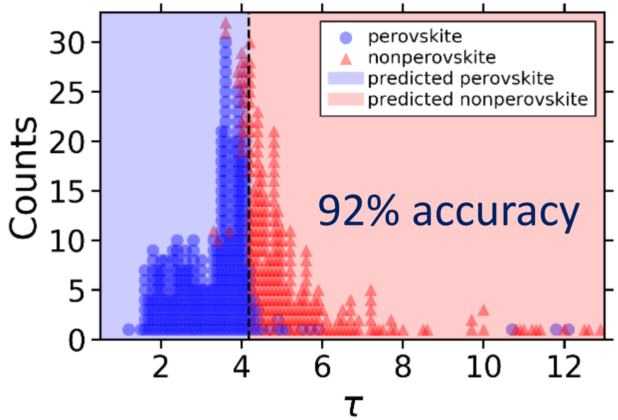
HydroGEN: Exciting Accomplishments

Solar Thermochemical H_2 Production

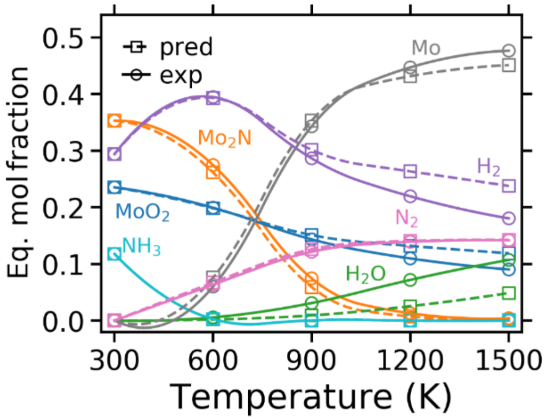
University of Colorado at Boulder: Utilized **Machine Learning** to rapidly screen ~10^{10} potential descriptors

- **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



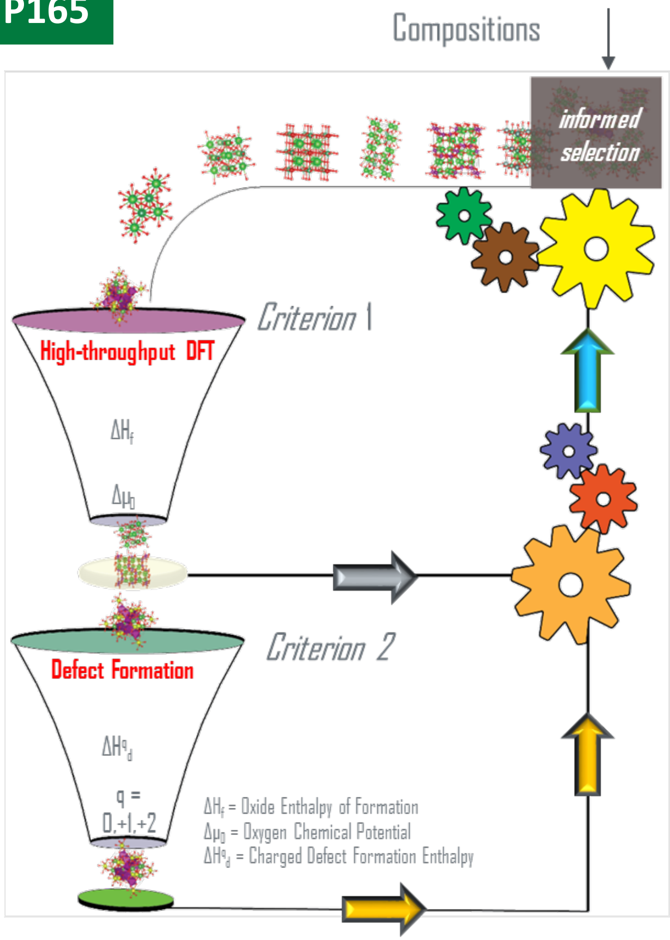
P166

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

HydroGEN: Exciting Accomplishments

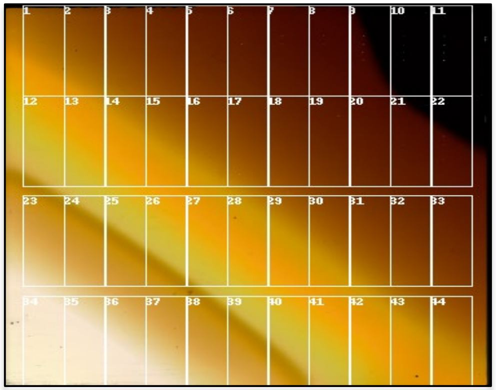
Solar Thermochemical H_2 Production

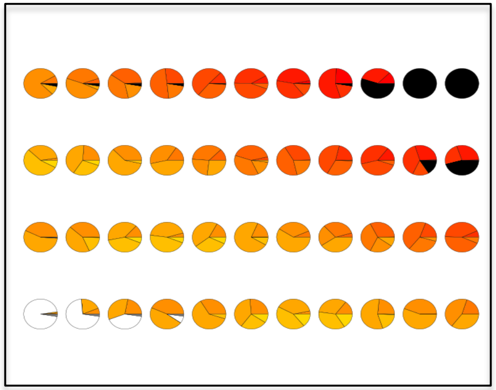
P165



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**





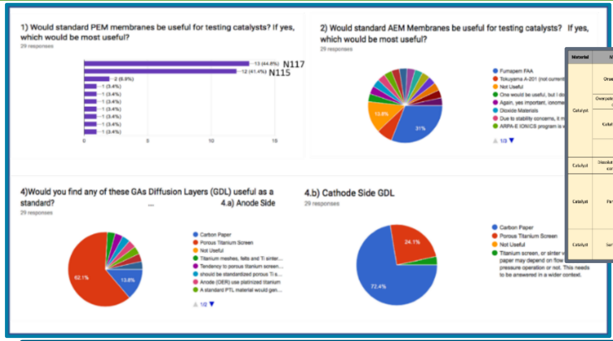
Machine learning, high-throughput and combinatorial approaches enabling accelerated STWS materials discovery

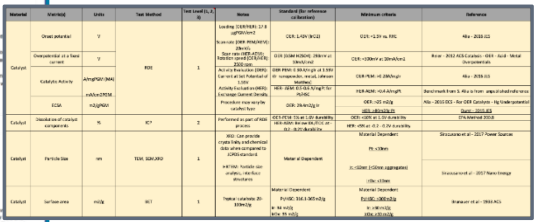
AWSM Best Practices and Protocol Development

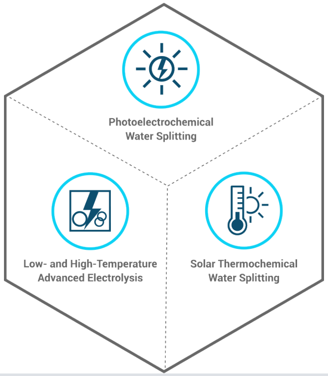
- **Framework** & **questionnaire** developed & distributed to broad, international community

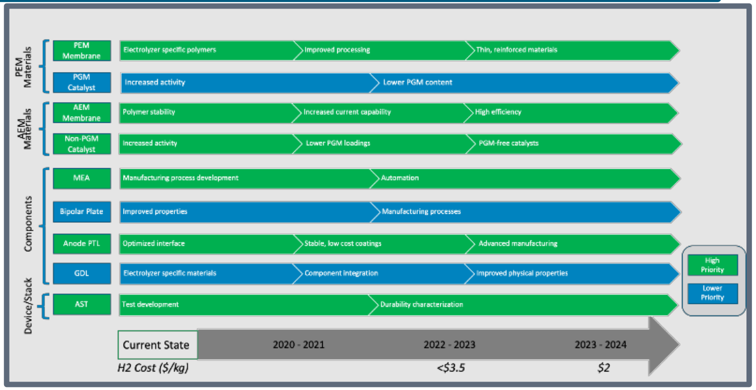
- **AWSM Workshop** to engage community & set priorities
  - > 80 experts representing 40 institutions across the AWSM community
  - Leveraging international efforts to increase harmony

- Preliminary **roadmaps** developed for each AWS technology









P170

AWSM Protocol Workshop held October 2018 at ASU

Hydrogen Fuel R&D Highlights

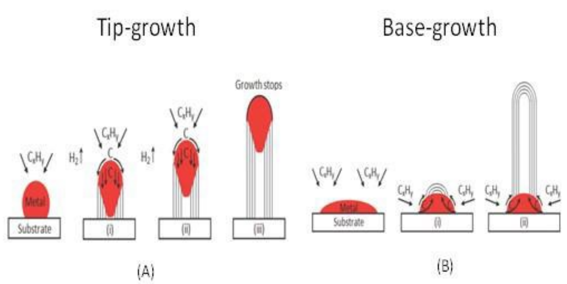
Innovative Concepts

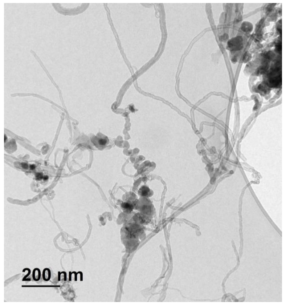
Solid Carbon

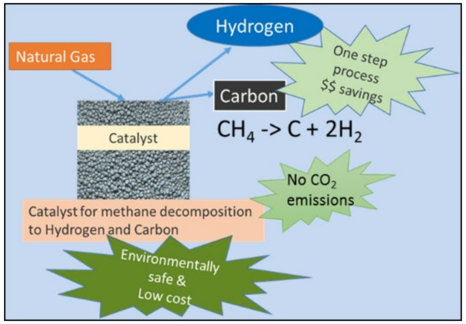
IA019

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_2-free H_2 and value added solid carbon materials.**







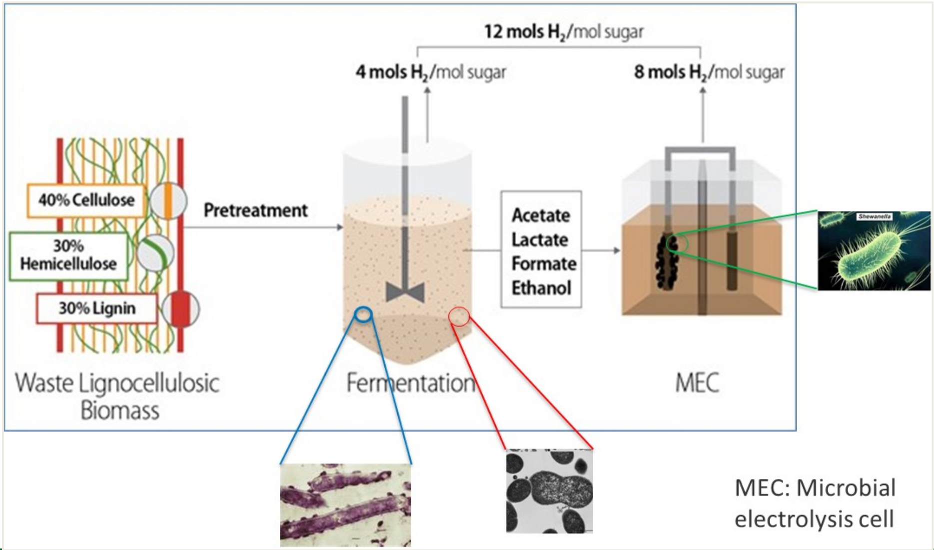
Biological H_2

P179

Initiated multi-Lab **BioH2 Consortium**

- **High-solid loading** fermentation technology to convert renewable biomass resources into H_2
- Integration with innovative microbial electrolysis cell (MEC) to **increase yield**

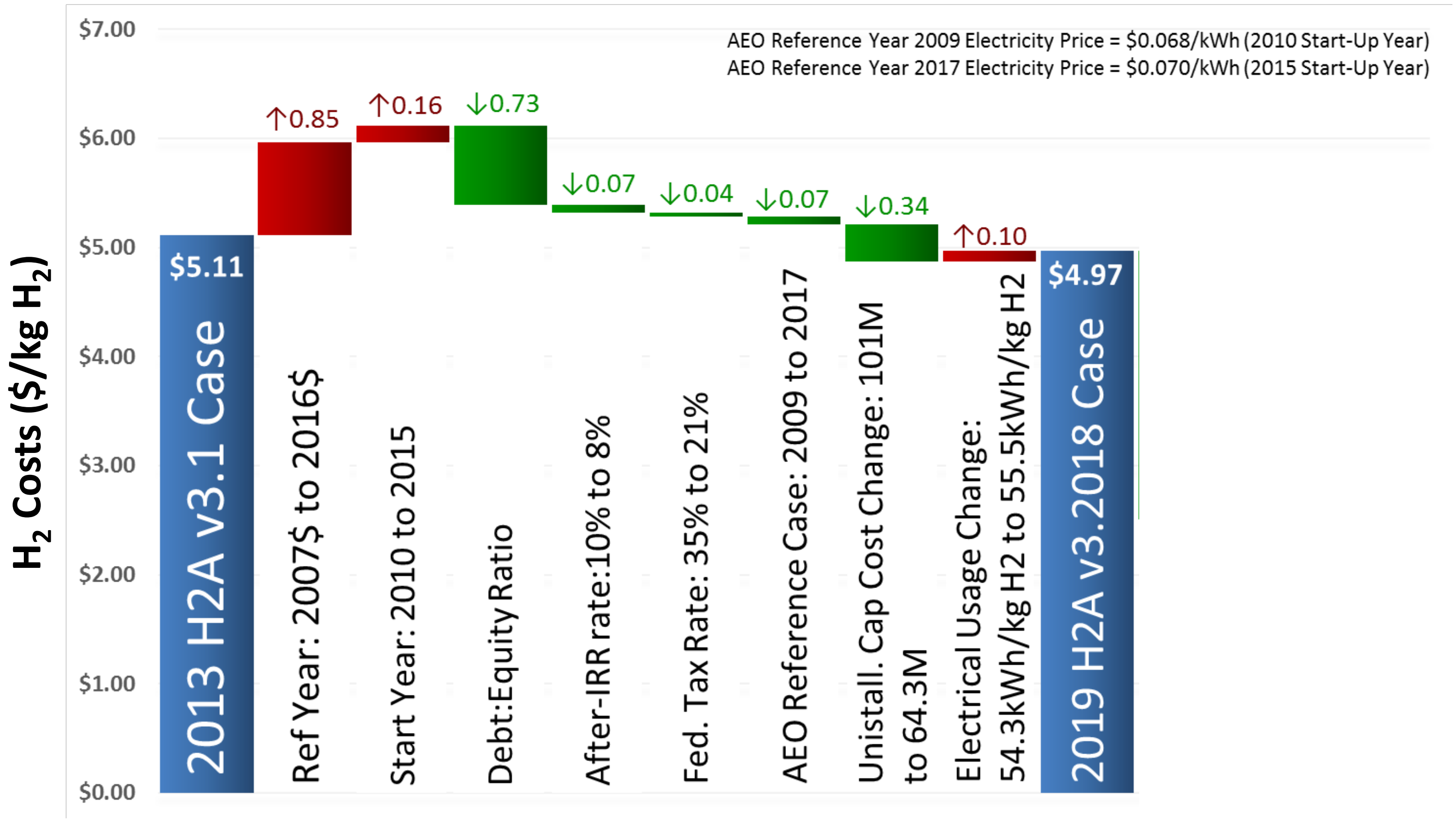
NREL NATIONAL RENEWABLE ENERGY LABORATORY · Pacific Northwest NATIONAL LABORATORY · BERKELEY LAB · Argonne NATIONAL LABORATORY · BioH2 Consortium



MEC: Microbial electrolysis cell

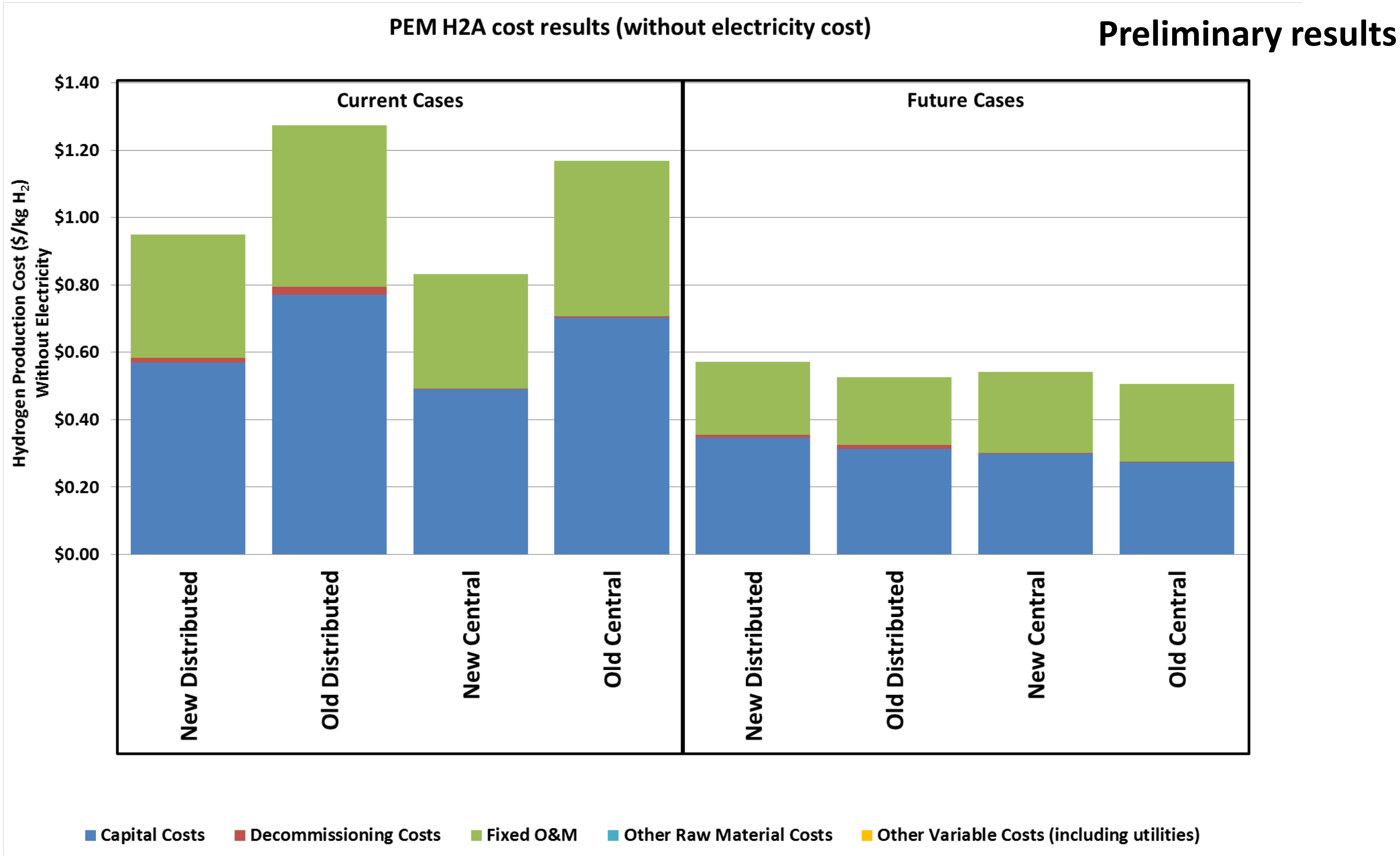
Updated cost analysis for LTE H_2 production

Current case – Preliminary results



Cost of H_2 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



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

Updated onboard storage cost record

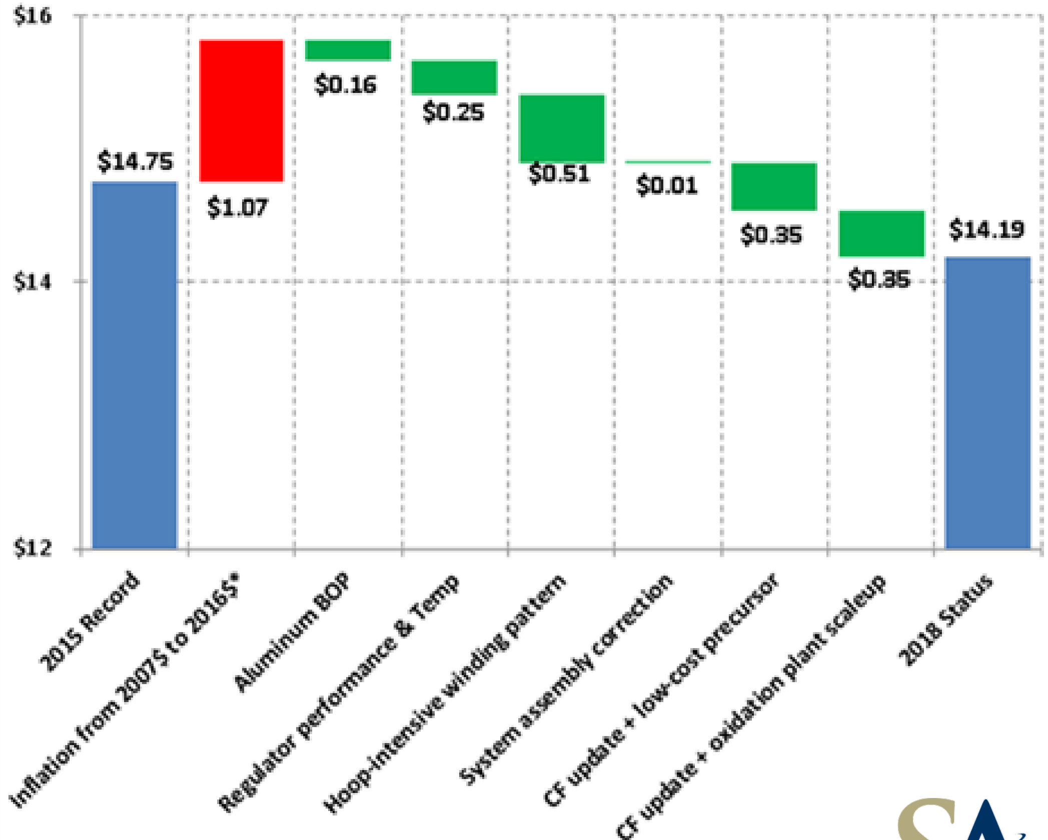
ST100

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



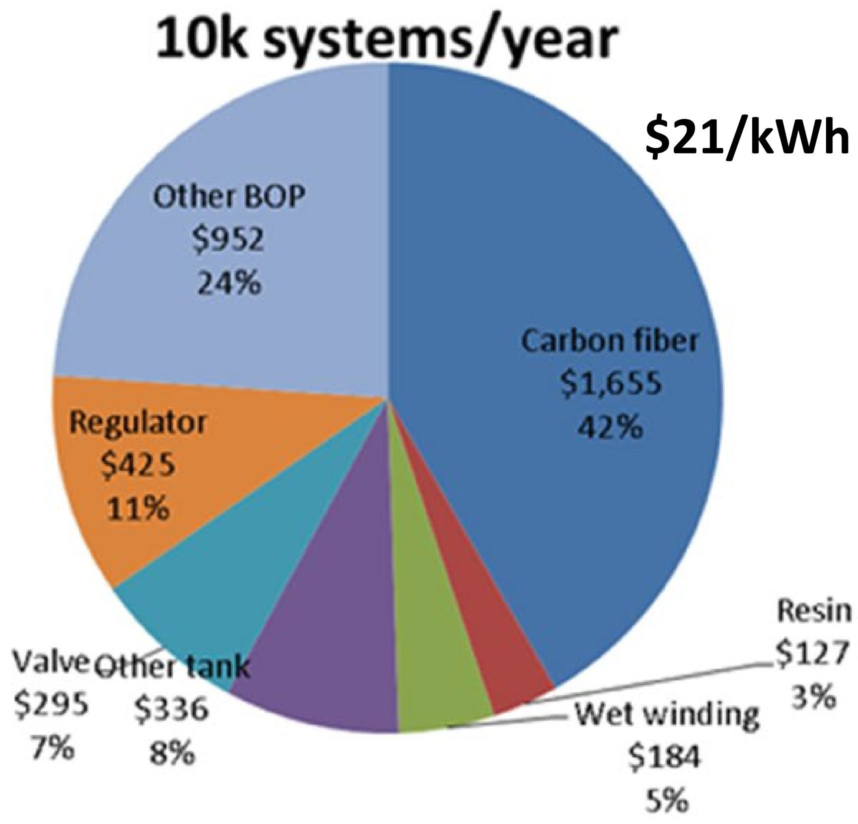
STRATEGIC ANALYSIS INC

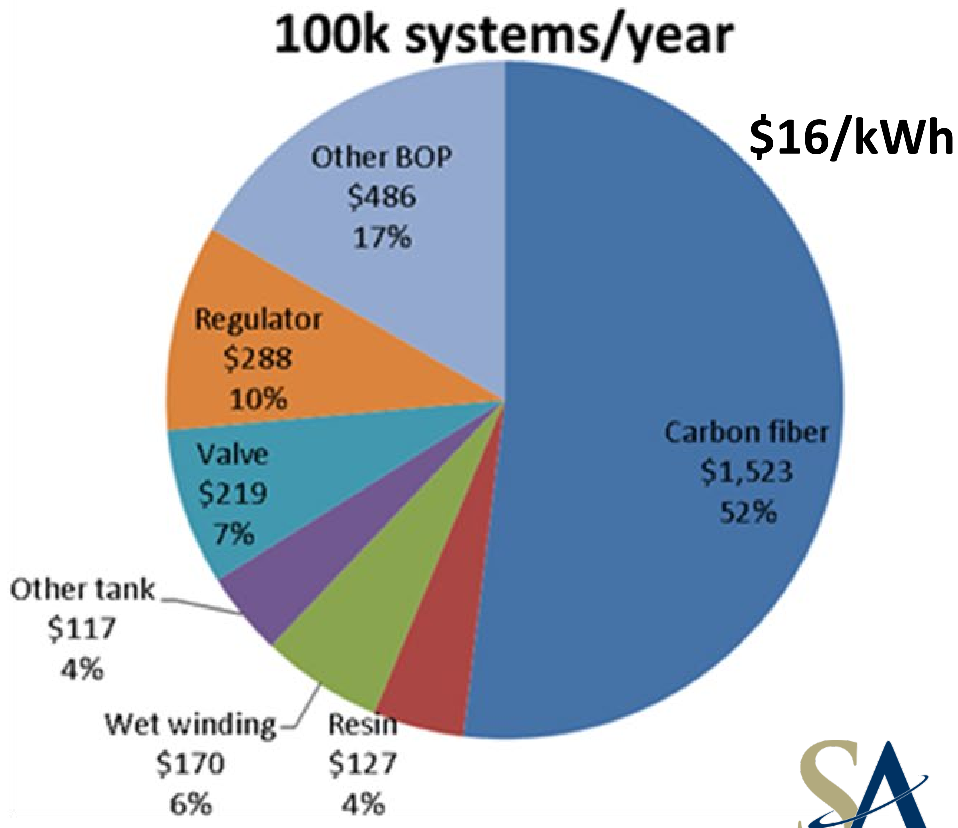
Improvements are continuously driving down costs, however costs are dominated by carbon fiber costs

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





STRATEGIC ANALYSIS INC

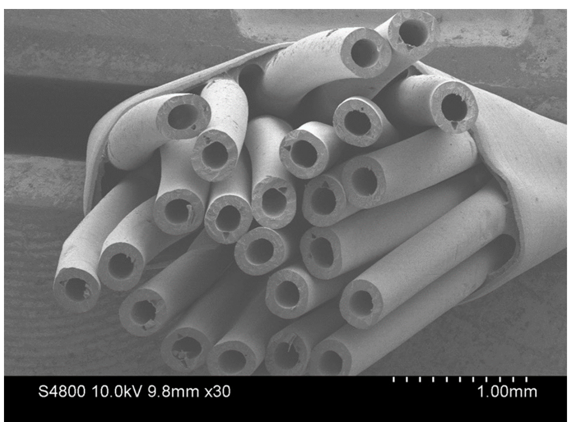
Single tank, 700 bar COPV onboard systems with 5.6 kg H_2 usable capacity

Reducing Carbon Fiber Cost through Precursors

Center for Applied Energy Research

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

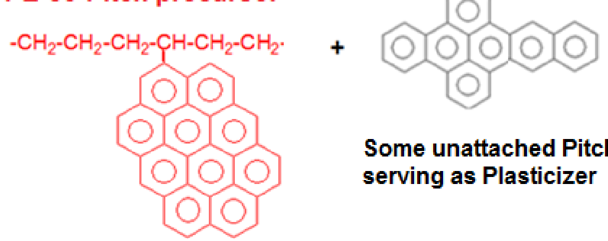


ST146

PENNSTATE

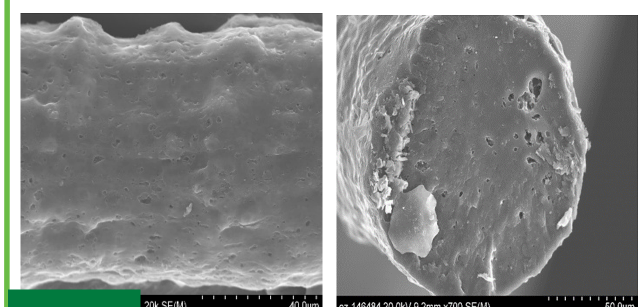
Development of low-cost polyolefin precursor fibers with high mass yield

PE-co-Pitch precursor



Some unattached Pitch serving as Plasticizer

> 70% mass yield demonstrated on carbonization

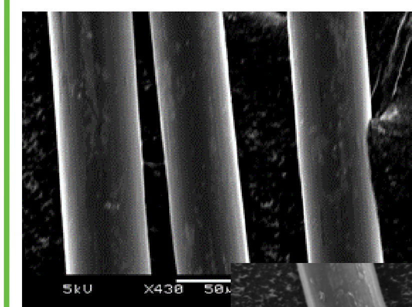


ST147

OAK RIDGE National Laboratory

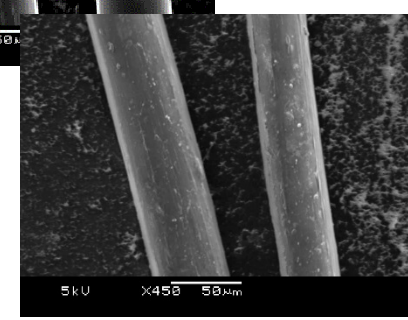
Novel plasticized PAN fibers produced through low-cost melt spinning

Ionic liquid	PAN (%)	As Spun Diameters (µm)	Washed Fiber Diameters (µm)
$[C_3mim]Br$	30	56.2 +/- 0.16	53.4 ± 7.6
$[C_4mim]Br$	30	56.8 +/- 0.20	45.6 ± 7.9
$[C_4mim]Cl$	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



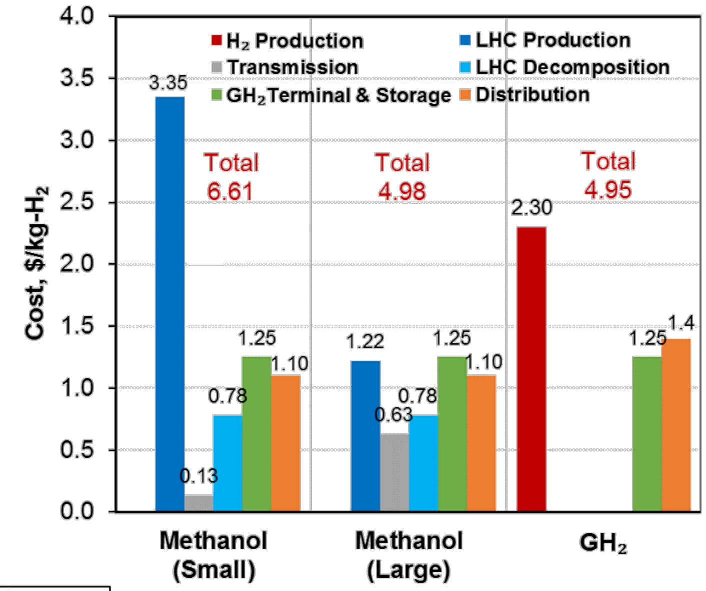
ST148

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

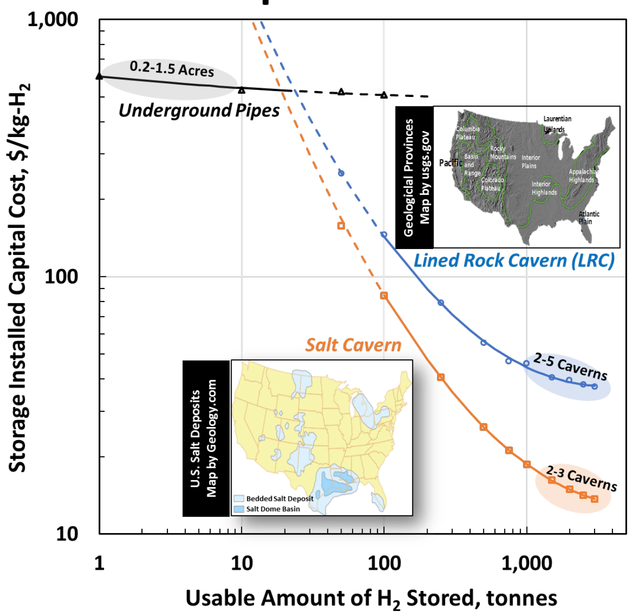
Technologies for transport and bulk storage

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

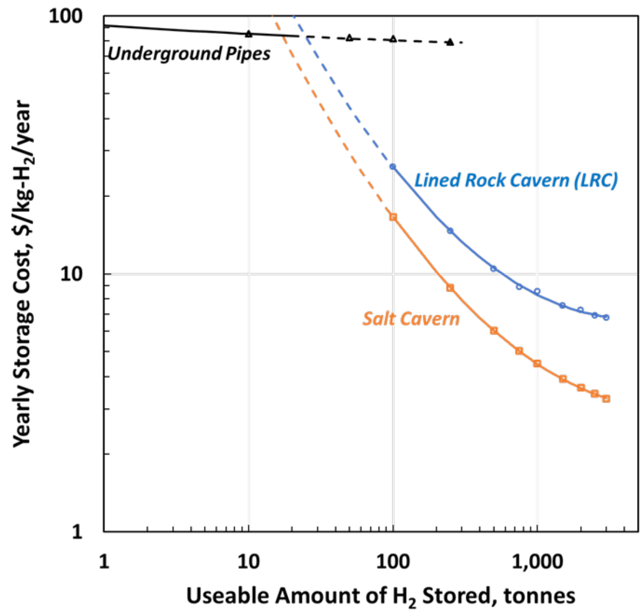
- 50 tonne per day H_2 usage
  - MCH, NH_3, and MeOH base cases
  - MeOH competitive with compressed H_2 even when transported 3000 km from gulf coast
- 500 tonne (10 day) bulk storage
  - Underground pipe, lined rock caverns and salt dome geologic storage base cases



Capital costs



Annual costs



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

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ST001

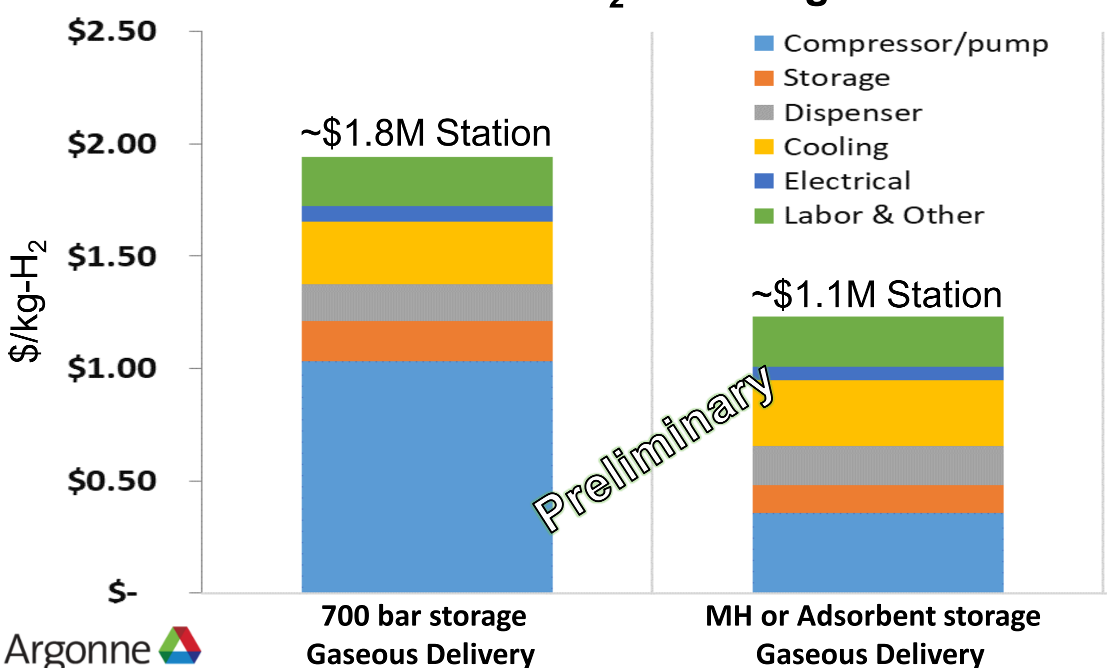
Hydrogen Interface Taskforce (H_2IT)

Cross TT taskforce developing a holistic H_2 pathway analysis across emerging H_2 production, delivery & onboard storage technologies

Storage System	Operating Temperature	Operating Pressure
700 bar Compressed H_2	Ambient (-40 to 85°C)	5 bar to 875 bar
Metal hydride (MH) or Adsorbent	Near ambient to 120°C	5 to 100 bar

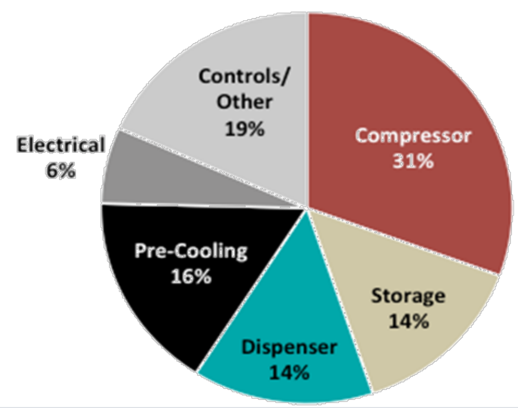
Assumptions:
- Sacramento, 50,000 FCEVs (~2030), [2016$]
- 37 HRS (1000 kg/day capacity)
- Manufacturing volume/learning
- Truck delivery (500 bar)

Contributions to H_2 Refueling Cost



- **~40% H_2 cost reduction**
- **~40% station cost reduction**
- **Reduces burden at station (less compression / precooling)**
- **Improved station reliability**

70 MPa station cost distribution



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SA170

Low-pressure, materials-based onboard storage enables lower H_2 & 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_2 Fuel R&D

- Navy - NUWC – materials-based storage for H_2-FC UUV applications
- Army – DEVCOM C5ISR – developing alane (AlH_3) production capacity
- Army – CCDC GVSC – onboard H_2 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_2 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_2 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_2 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