H₂ 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

**H₂ Fuel R&D Program consolidates the Production and Storage sub-programs**

**Senior Advisor**
Eric Miller

**Hydrogen Fuel R&D Program Manager**
Ned Stetson

**Technology Managers**
- Katie Randolph (Production Lead)
- Jesse Adams (Storage Lead)
- Bahman Habibzadeh
- New Fed 1
- New Fed 2

**Fuel Cells R&D Program Manager**
Dimitrios Papageorgopoulos

**Technology Managers**
- Donna Ho
- Greg Kleen
- Dave Peterson*

**Infrastructure & Systems R&D Program Manager**
Fred Joseck

**Technology Acceleration**
- Pete Devlin
- Nancy Garland*
- Jason Marcinkoski*
- Brian Hunter (AMO)
- Michael Hahn (WIND)

**Safety, Codes & Standards**
- Laura Hill
- Anthony Belvin (NNSA)

**Systems Analysis**
- Neha Rustagi (Delivery Lead) *
- Shawna McQueen

**Director**
Sunita Satyapal

**Operations**
Priya Swamy (BTO)

* 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
Advanced water-splitting materials

Innovative Concepts
Ex.: Leveraging biomass/waste for H₂ 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
Enabling twice the energy density for onboard H₂ 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 H₂ Fuel Portfolio helps enable
Cost Targets and Status

Production, Delivery & Dispensing

- Ultimate Targets:
  - High-Volume Projection: $16/gge*
  - Low-Volume Estimate: $13/gge

- High-Volume Projection (100K/yr):
  - $10/gge* to $5/gge**

- Low-Volume Estimate (500K/yr):
  - <$4/gge

Onboard Storage

- Ultimate Targets:
  - $16/kWh

- High-Volume Projection:
  - $21/kWh

- Low-Volume Estimate:
  - $8/kWh

Notes:
- Graphs not drawn to scale and are for illustration purposes only.
- gge: gallon of gasoline equivalent
- Storage costs based on preliminary 2019 storage cost record

† 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
Strategies: $H_2$ Production R&D

Continued Innovation is Needed across the Spectrum of Options

Applied Early-Stage R&D Needs

- Coal Gasification with CCUS
- Biomass Processing
- Natural Gas Conversion
- Waste to Energy
- Low Temp. Electrolysis
- High Temp. Electrolysis
- Direct-Solar

Widespread Adoption Timeline

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: H₂ Storage R&D

- **Off-board Focus Areas**
  - H₂ 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

**Widespread Adoption Timeline**

- **Salt Dome / Hard Rock Geologic**
- **Low to Moderate Pressure Compressed**
- **700 bar Type 3 & 4**
- **Cold/Cryo-Compressed**
- **Low Pressure Material-Based**

**Continued Innovation is Needed for both Onboard & Off-Board Storage**
Addressing Priorities: 2 FOAs with H$_2$ Fuel R&D Topics

**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)

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

• H₂ 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
H-Mat Consortium

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

Collaboration across Infrastructure, H₂ 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

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°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

5% increase in ILSS
HyMARC
HyMARC: Accelerating the development of viable hydrogen storage materials

Enabling twice the energy density for hydrogen storage

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

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

Individual Seedling Projects

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**  
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)

**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

**Focus Areas**

**User Facility POCs**

[Images of facility logos: ALS, SLAC, NREL, NIST, EMSL, Molecular Foundry]
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
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$_2$–10 mol% X + H$_2$  \[\xrightarrow{<200 \text{ bar}}\]  Mg(BH$_4$)$_2$ \[\xrightarrow{<250 \text{ °C}}\]

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.

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(BH₄)₂

Desorption plots for nano-encapsulated Mg(BH₄)₂

ALD nitride coated Mg(BH₄)₂ nanoparticles shown to have rapid desorption kinetics at relatively low temperatures (*NREL seedling*)

ALD Nitrides: High capacity Fast Kinetics

50 nm

ST143
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

Plasmonic photocatalysts shown to have potential to effect room temp H$_2$ release
Pioneering Research in Water Splitting

- 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
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$_4$CeMn$_3$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

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
**H₂ Production: Exciting Accomplishments**

**High Temperature Electrolysis**

**FuelCell Energy** demonstrated 45 cell SOEC stack with virtually **no degradation over ~4000 hr** at 1 A/cm² with **>95% electrical efficiency**

![Graph showing cell voltage over elapsed time]

-1 A/cm²: 3.3 kg/d H₂ production
-1.22 A/cm²: 4 kg/d H₂ production

>4 kg H₂/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**
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/cm² at 1.8 V (testing at Giner)

PGM-free electrodes demonstrating reasonable current densities in MEAs at typical cell operating voltages
Northeastern University demonstrated continued performance improvement for completely PGM-free AEM electrolysis with advanced catalysts and membranes:

- Achieved current density of 800 mA/cm² 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.
Rutgers demonstrated a:

- **Bioinspired** high solar-to-hydrogen efficiency system
- **11.5% with PGM-free** Ni$_5$P$_4$ 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!
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!
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

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Machine learning, high-throughput and combinatorial approaches enable accelerated STWS materials discovery
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
  o > 80 experts representing 40 institutions across the AWSM community
  o Leveraging international efforts to increase harmony

• Preliminary roadmaps developed for each AWS technology

AWSM Protocol Workshop held October 2018 at ASU
Hydrogen Fuel R&D Highlights
Innovative Concepts

Solid Carbon

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\textsubscript{2}-free H\textsubscript{2} and value added solid carbon materials.

Biological H\textsubscript{2}

Initiated multi-Lab BioH\textsubscript{2} Consortium

- **High-solid loading** fermentation technology to convert renewable biomass resources into H\textsubscript{2}
- Integration with innovative microbial electrolysis cell (MEC) to *increase yield*

**MEC: Microbial electrolysis cell**
Updated cost analysis for LTE H₂ production

Current case – Preliminary results

Cost of H₂ production by low-temperature PEM electrolysis updated to reflect current assumptions and realities – net result – *slight reduction in cost*
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 dominate the cost of 700 bar COPV systems, however significant cost reductions still can be made in BOP components.

Single tank, 700 bar COPV onboard systems with 5.6 kg H₂ 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

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

- PE-co-Pitch precursor
  - \( \text{CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-} \)

  \[ \text{Some unattached Pitch serving as Plasticizer} \]

  > 70% mass yield demonstrated on carbonization

Novel plasticized PAN fibers produced through low-cost melt spinning

<table>
<thead>
<tr>
<th>Ionic liquid</th>
<th>PAN (%)</th>
<th>As Spun Diameters (µm)</th>
<th>Washed Fiber Diameters (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[C₅mim]Br</td>
<td>30</td>
<td>56.2 +/- 0.16</td>
<td>53.4 ± 7.6</td>
</tr>
<tr>
<td>[C₅mim]Br</td>
<td>30</td>
<td>56.8 +/- 0.20</td>
<td>45.6 ± 7.9</td>
</tr>
<tr>
<td>[C₅mim]Cl</td>
<td>30</td>
<td>54.7 +/- 0.08</td>
<td>45.3 ± 8.7</td>
</tr>
<tr>
<td>[MPCNIm]Br</td>
<td>30</td>
<td>59.6 +/- 0.25</td>
<td>47.9 ± 14.1</td>
</tr>
<tr>
<td>[MPCNIm]Cl</td>
<td>30</td>
<td>53.4 +/- 0.17</td>
<td>48.6 ± 10.4</td>
</tr>
</tbody>
</table>

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 H₂ usage
- MCH, NH₃, and MeOH base cases
- MeOH competitive with compressed H₂ 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

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.
Hydrogen Interface Taskforce (H₂IT)

Cross TT taskforce developing a holistic H₂ pathway analysis across emerging H₂ production, delivery & onboard storage technologies

<table>
<thead>
<tr>
<th>Storage System</th>
<th>Operating Temperature</th>
<th>Operating Pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>700 bar Compressed H₂</td>
<td>Ambient (-40 to 85°C)</td>
<td>5 bar to 875 bar</td>
</tr>
<tr>
<td>Metal hydride (MH) or Adsorbent</td>
<td>Near ambient to 120°C</td>
<td>5 to 100 bar</td>
</tr>
</tbody>
</table>

Contributions to H₂ Refueling Cost

- ~40% H₂ cost reduction
- ~40% station cost reduction
- Reduces burden at station (less compression / precooling)
- Improved station reliability

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

Low-pressure, materials-based onboard storage enables lower H₂ & station costs
Interagency Collaborations

Collaborations between NSF projects and FCTO EMN consortia
- NSF-DMREF / HydroGEN EMN
- NSF-SSMC / HyMARC EMN

Collaborations between DOD and FCTO H₂ Fuel R&D
- Navy - NUWC – materials-based storage for H₂-FC UUV applications
- Army – DEVCOM C5ISR – developing alane (AlH₃) production capacity
- Army – CCDC GVSC – onboard H₂ storage for combat vehicles

Collaborations between DOC projects and FCTO EMN consortia
- NIST Center for Neutron Research / HyMARC EMN

Interagency Collaborations

Collaborations between FCTO H₂ 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
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Thank you from the Hydrogen Fuel R&D Team

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