HydroGEN Overview: A Consortium on Advanced Water Splitting Materials

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Presenter: Huyen Dinh, NREL
Date: 5/20/2020
Venue: 2020 DOE Annual Merit Review

This presentation does not contain any proprietary, confidential, or otherwise restricted information.
HydroGEN Overview

Timeline and Budget

• Start date (launch): June 2016
• FY17 DOE funding: $3.5M
• FY18 DOE funding: $9.9M
• FY19 DOE funding: $8.4M
• FY20 planned DOE funding: $10.6M
• Total DOE funding received to date: $30M

Barriers

• Cost
• Efficiency
• Durability

Partners
Collaboration: HydroGEN Steering Committee

Huyen Dinh (Director)

Adam Weber (Deputy Director)

Anthony McDaniel (Deputy Director)

Richard Boardman

Tadashi Ogitsu

Elise Fox

Ned Stetson and Katie Randolph, DOE-EERE-FCTO
HydroGEN: Advanced Water Splitting Materials

Materials innovations are key to enhancing performance, durability, and cost of hydrogen generation, storage, distribution, and utilization technologies key to H2@Scale

Large-scale, low-cost hydrogen from diverse domestic resources enables an economically competitive and environmentally beneficial future energy system across sectors.


*Illustrative example, not comprehensive*
Energy Materials Network (EMN)
Relevance and Impact

DOE’s EMN aims to accelerate early-stage applied R&D in materials tracks aligned with some of the nation’s most pressing sustainable energy challenges.

- Hydrogen Compatible Materials
- Breakthrough Hydrogen Storage Materials
- Advanced Water Splitting Materials for Hydrogen Production
- Next-Generation Electro-catalysts for Fuel Cells

example tracks

Accelerating early-stage materials R&D for energy applications
Advanced Water-Splitting Materials (AWSM) Relevance, Overall Objective, Impact, and Approach

Accelerating R&D of innovative materials critical to advanced water splitting technologies for clean, sustainable, and low cost H₂ production, including:

- Photoelectrochemical (PEC)
- Solar Thermochemical (STCH)
- Low- and High-Temperature Advanced Electrolysis (LTE & HTE)

H₂ Production target <$2/kg

HydroGEN consortium supports early stage R&D in H₂ production
HydroGEN fosters cross-cutting innovation using theory-guided applied materials R&D to advance all emerging water-splitting pathways for hydrogen production

Website: https://www.h2awsm.org/
Approach/Collaboration: HydroGEN EMN

HydroGEN Nodes

Lab-led R&D: Supernode (cross-lab collaboration)

Lab – FOA Projects

Multi-Agency Projects

Best Practices in Materials Characterization and Benchmarking

Data Hub

AWS Research Community
**Accomplishments: Developed New Publication Search Engine and Updated Capability Nodes**

Developed **dynamic publications list** that pulls directly from **H2AWSM Zotero library**

- Phase 1 (2020): HydroGEN publications and presentations
- Phase 2 (Future): All water-splitting literature resources

**Added 1 new, updated >10 current, and removed 2 capability nodes**

- **New**: Microelectrode Testing of LTE Electrocatalysts, Ionomers, and Their Interactions in the Solid State

**View publication details and access DOI or PDF link**

**Filter by type, year, AWS technology, and Zotero tags**

**Annual capability review is a rigorous process and keeps nodes updated and relevant**

[https://www.h2awsm.org/publications](https://www.h2awsm.org/publications)
Accomplishments: Maintained HydroGEN Website and Participated in MRS TV Video

MRS TV Video
- Featured interviews and footage from across HydroGEN
- Broadcast at 2019 MRS Fall Meeting
- 3,137 views on MRS TV website
- Also posted on HydroGEN and DOE FCTO websites
- Raw footage can be used in additional consortium videos

Video can be found here: https://youtu.be/PUti7ku2_ig

h2awsm.org

5,407 users
7,353 sessions
23,382 pageviews
445 file downloads
629 video clicks

Traffic:
- 54% search
- 27% direct
- 18% referral

Top Pages:
- Home
- Capabilities

HydroGEN: Advanced Water Splitting Materials
Accomplishments:
HydroGEN Data Hub: Making Digital Data Accessible

https://datahub.h2awsm.org/

User 179 → 258 (↑ 44%)
Files 4,055 → 36,580 (↑ 8000%)
Public Datasets: 21

Data Hub 2019-2020 Year in Review
• Grew Data Hub community and site visits
• Implemented data governance processes
• Upgraded Data Hub software platform
• Expanded visualization of multi-spectra data
• Developed metadata for each AWS technology
• Metadata endpoints – data curation, improved upload.

Growing and active user community

Many Types of Experimental Data
Material characterization
• XRD, SFR, XPS, XRF, SEM, TEM, Raman,
Device performance
• Electrolysis, PEC J-V, IPCE, Tafel plots,
Materials durability data
• TGA, membrane conductivity

Assigning a Digital Object Identifier (DOI) to public datasets for a persistent landing page and scientific discovery.

Cumulative Data Added
User Percentage
May 2017
March 2020

HydroGEN: Advanced Water Splitting Materials

XRD = x-ray diffraction; SFR = stagnation flow reactor; J-V = current vs. voltage data; TEM = transmission electron microscopy
XPS = x-ray photoelectron spectroscopy; TGA = thermal gravimetric analysis; IPCE = incident photon to current efficiency

Other = Raman spectroscopy, rheology, helium ion microscope images, conductivity, dilatometry, kinetic, XRF

Data Team
Accomplishments: Data Hub Metrics and Data Governance

Data Hub Metrics: Tracking Access and Utilization

- 414 Data Hub visits from outside the United States
- 2,387 visits from within the United States
- 786 sessions are from users logging in to contribute to private data within projects.

Data Governance for Availability, Usability, Integrity and Security

New User Resources include:

- Metadata API endpoints
- Updated data release procedure
- Project closeout procedure
- Zotero tutorial
- Terms and privacy policy

- FAIR data standard
- Better data quality and usability
- Increased availability and accessibility

April 2019–April 2020
Accomplishments: Data Tools for Visualization and Analysis: Multi-Spectra and Phase and Defect Formation Diagram

The interactive **Advanced Multi-Spectra Data View** allows many spectra files (any csv or tabular file format) to be visualized at one time, from one or many files.


LLNL developed the dynamic GUI for **Defect Analysis** that generates the defect stability plot (right) for a given alloy composition (left: click a point in alloy phase diagram), and NREL implemented it on the Data Hub for photoabsorber (PEC) and STCH materials development.

Accomplishments: Metadata Automation and Standardization

Metadata is crucial to efficient utilization of stored data

- Capture all information about source, experiment, computation, sample, measurement, and result
  - Enable powerful searching across datasets
- Automate metadata capture and upload/download tasks
  - Standard templates
  - GUI-based framework
  - User-friendly and error-free
- Python parsing architecture facilitates customization
- Shared code in Github facilitates collaboration

HydroGEN Data Hub

- Tabular data (Excel, CVS) with embedded metadata
- STCH, LTE, HTE, PEC data
- Other data types...

Common framework

GUI driven uploader

Rich, standard metadata connected to data
Accomplishments: Technology Transfer Agreements (TT/A)

Streamlined Access

- **Four** standard, pre-approved TT/A between all consortium partners
  - Non-Disclosure Agreement (NDA)
  - Intellectual Property Management Plan (IPMP)
  - Materials Transfer Agreement (MTA)
  - Cooperative Research and Development Agreement (CRADA)
- Updated NDA
- Executed all 33 project NDAs

Non-Disclosure Agreement (NDA)

- Information Disclosure

Intellectual Property Management Plan (IPMP)

- IP Protection

Materials Transfer Agreement (MTA)

- Freedom to Operate

Cooperative Research and Development Agreement (CRADA)

- Collaboration

https://www.h2awsm.org/working-with-hydrogen
HydroGEN is vastly collaborative, has produced many high value products, and is disseminating them to the R&D community.
Interagency collaboration enables development of an integrated membrane database with new schema and dissemination
DMREF – HydroGEN Collaboration

**Goal:** Accelerate Pt-free ternary photocatalysts $M_xV_2O_5/CdX/MoS_2$ for solar hydrogen generation

**Collaboration Achievements:** Integrating MoS$_2$ co-catalysts to rationally designed photocatalysts

A. Parija et al., ACS Cent. Sci. 2018, 4, 4, 493-503

Banerjee, Watson, Piper, to be submitted

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**Collaboration: Material Discovery & Advanced**

1. Increase Foundry of Nanocomposite Photocatalysts
2. Develop Pt-free co-catalysts
3. Adapt In-situ X-ray Characterization
4. Perform X-ray simulations

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Leveraging HydroGEN advanced characterization and modeling enabled deeper understanding of photocatalysts for solar hydrogen generation; accelerating the design of novel third-generation ternary heterostructured catalysts
Experiments confirm favorable redox alignment and hydrogen generation for 9 of the 14 synthesized compounds, with the most promising ones belonging to the families of alkali and alkaline-earth indates and plumbates.
Collaboration Goal: Leverage non-oxide (DMREF) and oxide (HydroGEN EMN) defect calculations to build a comprehensive database of defect calculations.

Impact: Creation of a central repository of defect calculations that will allow data informatics approaches for predicting dopability.

Lessons: To build reliable machine learning (ML) models, need for diverse (composition, structure) dataset; possible by leveraging multiple projects.
Collaboration: HydroGEN FOA-Awarded Projects

31 FOA-Awarded Projects

43 unique capabilities being utilized across six core labs

<table>
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<th>Advanced Electrolysis (16)</th>
<th>PEC (7)</th>
<th>STCH (7)</th>
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<td>LTE (8)</td>
<td>Benchmarking &amp; Protocols (1)</td>
<td>2-Step MO$_x$ (6)</td>
</tr>
<tr>
<td>HTE (8)</td>
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<td>Hybrid Cycle (1)</td>
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## A Balanced AWSM R&D Portfolio Approach/Collaboration

### Low Temperature Electrolysis (LTE)
(G. Bender: P148C; 8 Projects)

**PEM Electrolysis**
- PEM Component Integration
  - PEM electrolysis

**AEM Electrolysis**
- • PGM-free OER and HER catalyst
- • Novel AEM and Ionomers
- • Electrodes

### High Temperature Electrolysis (HTE)
(G. Groenewold: P148D; 8 Projects)

**O₂⁻ conducting SOEC**
- • Degradation mechanism at high current density operation
- • Nickelate-based electrode and scalable, all-ceramic stack design
- • Neodymium and lanthanum nickelate

**H⁺ conducting SOEC**
- • High performing and durable electrocatalysts
- • Electrolyte and electrodes
- • Low cost electrolyte deposition
- • Metal supported cells

### Photoelectrochemical (PEC)
(N. Danilovic: P148A; 7 Projects)

**Semiconductors**
- • III-V and Si-based semiconductors
- • Chalcopyrites
- • Thin-film/Si
- • Protective catalyst system
- • Tandem cell

**Perovskites**
- • PGM-free catalyst
- • Earth abundant catalysts
- • Layered 2D perovskites
- • Tandem junction

### Solar Thermochemical (STCH)
(A. McDaniel: P148B; 7 Projects)

**STCH**
- • Computation-driven discovery and experimental demonstration of STCH materials
- • Perovskites, metal oxides

**Hybrid Thermochemical**
- • Solar driven sulfur-based process (HyS)
- • Reactor catalyst material

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PEM = proton exchange membrane electrolysis; AEM = alkaline exchange membrane electrolysis

PGM = platinum group metal

Solid oxide electrolysis cells: SOEC
Collaboration: Top HydroGEN Capability Nodes By Project Utilization (LTE, HTE, PEC, STCH projects)

<table>
<thead>
<tr>
<th>HydroGEN Capability Node</th>
<th>Node Class</th>
<th>LTE</th>
<th>HTE</th>
<th>PEC</th>
<th>STCH</th>
</tr>
</thead>
<tbody>
<tr>
<td>LBNL Multiscale Modeling of Water Splitting Devices</td>
<td>Modeling</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>INL Advanced Materials for Elevated Temperature Water Electrolysis</td>
<td>Characterization</td>
<td>9</td>
<td></td>
<td>9</td>
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</tr>
<tr>
<td>NREL In-Situ Testing Capabilities for Hydrogen Generation</td>
<td>Characterization</td>
<td></td>
<td>8</td>
<td>9</td>
<td></td>
</tr>
<tr>
<td>NREL Thin Film Combinatorial Capabilities for Advanced Water Splitting Technologies</td>
<td>Synthesis + Characterization</td>
<td>3</td>
<td>2</td>
<td>2</td>
<td></td>
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<tr>
<td>NREL First Principles Materials Theory for Advanced Water Splitting Pathways</td>
<td>Modeling</td>
<td></td>
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<td></td>
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<tr>
<td>NREL On-Sun PEC Solar-to-Hydrogen Benchmarking</td>
<td>Characterization</td>
<td></td>
<td>6</td>
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<td></td>
</tr>
<tr>
<td>LBNL Thin Film and Bulk Ionomer Characterization</td>
<td>Characterization</td>
<td></td>
<td>6</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SNL High-Temperature X-ray Diffraction and Thermal Analysis</td>
<td>Characterization</td>
<td></td>
<td></td>
<td>1</td>
<td>5</td>
</tr>
<tr>
<td>NREL Multi-Component Ink Development, High Throughput Fabrication, and Scaling Studies</td>
<td>Processing &amp; Scale Up</td>
<td>5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SNL Virtually Accessible Laser Heated Stagnation Flow Reactor</td>
<td>Characterization</td>
<td></td>
<td></td>
<td></td>
<td>5</td>
</tr>
<tr>
<td>LLNL Ab Initio Modeling of Electrochemical Interfaces</td>
<td>Modeling</td>
<td>4</td>
<td></td>
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HydroGEN characterization capability nodes are the most utilized by projects across different AWS technologies.
Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

**Low Temperature Electrolysis (LTE)**
LANL, Rensselaer Polytechnic Institute, and Nel demonstrated high AEM electrolyzer performance that approaches the 2020 target (2 A/cm² at 1.8 V, 60°C) using polystyrene based alkaline polymers that are durable and economically affordable. SNL provided control AEM and ionomer and NREL nodes studied the effect of pH on AEM performance. LBNL modeling and characterization nodes helped LANL better understand the ionomer stability, ionomer/catalyst interface, and pH effect.

**Photoelectrochemical (PEC) Water Splitting**
University of Hawaii extended chalcopyrites durability to 270 hours using atomic layer deposition (ALD) WO₃ coatings, paving the way to creating a low cost (“printed”) chalcopyrite-based, semi-monolithic, tandem hybrid photoelectrode device prototype that can operate for at least 1,000 h with solar-to-hydrogen efficiency >10%. This project is supported by NREL synthesis and advanced characterization and LLNL modeling expertise to accelerate the development of materials and interfaces.
Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

High Temperature Electrolysis (HTE)
University of Connecticut, with INL, successfully developed a new triple-phase conducting oxide, PNC perovskite, as an oxygen electrode in proton conducting solid oxide electrolysis cells (H-SOEC), exhibiting good electrochemical performance at reduced temperatures of 400°–600°C. The electrolysis current density achieved (1.72 A/cm² at 1.4 V and 600°C) is the highest performance to date. Furthermore, H-SOECs with this electrode material showed robust durability for thermal cycling and reversible operation at these temperatures.

Solar Thermochemical (STCH) Water Splitting
Arizona State University (ASU) and Princeton computationally predicted, and NREL synthesized, a ternary oxide STCH material for water splitting that has the potential to achieve higher specific capacities and larger H₂ to H₂O ratios and meet the hydrogen production cost targets. These results point to the importance of both valence state and crystalline structure in achieving large degrees of reversible reduction and open the door to a new class of STCH materials.
Five New Supernodes: Accelerate AWSM Materials R&D through Lab Collaboration

Supernodes Objectives:

- Combine/integrate nodes to demonstrate value when connected (sum greater than combination of individual parts)
- Increase collaboration across core labs
- Provide core research for EMN labs, beyond just project support
1. LTE/Hybrid Supernode: Linking Low-Temperature Electrolysis (LTE)/Hybrid Materials to Electrode Properties to Performance (NREL, SRNL, LBNL; 8 Nodes)

Goals: Create true understanding between ex-situ and in-situ performance. Identify how material properties are linked to electrode properties and how these are linked to electrolyzer performance.

Outcome: Better integration between ex-situ and in-situ performance, more relevant ex-situ testing, and improved material specific component development to achieve optimized electrolyzer cell performance and durability.
1. LTE/Hybrid Supernode Accomplishments: RDE/MEA Correlation, Multiscale Modeling, and Scalable Coating Methods

Correlation between RDE and MEA systems confirmed for LTE and Hybrid Cycle

**LTE**

**Hybrid Cycle**

### Multiscale modeling agrees with experimental data

### Scalable coating methods (doctor blade) show comparable performance to lab-scale coatings (ultrasonic spray)


2. **OER Supernode**: Validated Multiscale Modeling To Understand OER Mechanisms across the pH Scale (NREL, LBNL; LLNL; 6 Nodes)

**Goal**: Utilize validated theory across length scales to understand the mechanism of oxygen evolution going from acid to neutral to alkaline pH. Provide critical analysis for both LTE and PEC technologies.

- **AP-XPS**: Surface intermediate coverage
- **Microelectrode**: $E_g$ and $\Delta G_{\text{rxn}}$ for each elementary step
- **RDE**: Species flux at catalyst surface
- **OER rates and mechanism**: Catalyst surface structure
- **DFT calculations**: Species activity near the catalyst
- **MD/DFT simulations**: Species activity near the catalyst
- **Microkinetic model**: Double-layer and solvent structure
- **Continuum transport**: Species concentration near double layer
- **Surface coverage**: Concentration profiles
2. OER Supernode Accomplishment: Applied Multi-Scale Theories to Model OER Mechanism across pH Scales and Validated Experimentally on IrO₂

**Atomistic Modeling (DFT, NREL)**
- Explore reaction mechanisms how to determine barriers

1. Bare Ir Surface
   - Low O coverage limit (multiple pathways)
   - High O coverage limit (thermodynamically favored)

2. IrO₂ Surface from Pourbaix Analysis
   - Established a way to determine intermediates, energetics and kinetics of OER
   - Improved *ab-initio* Pourbaix diagram
   - Refining transition states with *ab-initio* simulations
   - Method to examine effects of solvation established

**Microkinetic Modeling (LBNL)**
- Use barriers from DFT and MD calculations to model OER rate and pathways, including mass transports
- Good agreement for low pH
- Surface coverages

**Experimental RDE Results (NREL)**
- For Ir metal, activity improvement extended into weakly basic pH
- Activity dropped at pH 0/14, may be due to contaminants at higher concentrations
3. PEC Supernode: Emergent Degradation Mechanisms with Integration and Scale Up of PEC Devices (NREL, LBNL; 7 Nodes)

**Goal:** Understand integration issues and emergent degradation mechanisms of PEC devices at relevant scale and demonstrate an integrated and durable 50 cm² PEC panel.

- Benchmarking
- *In situ* degradation and characterization
- Emerging degradation pathways
- Modeling

![Diagram showing scale up of PEC devices](image)
3. PEC Supernode Accomplishments: Fabrication, Cell Design, and On Sun PEC Testing Scale Up

PEC Fabrication: GaInP/GaAs cells with 0.1 to 8-cm²

PV cells: ~0.1 cm² ~1 cm² 8 cm²

Scale Up Towards 8-cm² Illuminated Area

On Sun Durability Testing: 8-cm² Cell

- Test Duration: 2 days, 2 hours, and 50 minutes
- Steady-state STH efficiency was 9.2%

Degradation Modes Observed: 8-cm² Cell

- Gold grid finger delamination
- Anti-reflective coating dissolution
- Bubbles in epoxy – more light scattering
- Blistering

ICP-MS analysis of effluent showed Ga in cathode and 1-2 ppm Ir in anode
**4. HTE Supernode:** Characterization of Solid Oxide Electrode Microstructure Evolution (INL, NREL, LBNL, LLNL, Sandia; 7 Nodes)

**Goal:** Deeper understanding of high-temperature electrolysis (HTE) electrode microstructure evolution as a function of local solid oxide composition and operating conditions.

**Impact:** Comprehensive platform of HTE science and technology available for rapid utilization by HTE developers.

Need: integrated, diverse set of capabilities and expertise, coordinated to develop a comprehensive understanding of HTE

7 nodes combined: INL, NREL, LBNL, LLNL, SNL
4. HTE Supernode Accomplishment: Cell Quality Control, Synchrotron Characterization, and Multiscale Microstructure Modeling Framework

**Demonstrated quality control of R2R cell fabrication process (5 layers in cell) (INL)**

- Confirmed reproducibility of phase purity (XRD), structure (SEM) and SOEC performance of YSZ-based reference cells

**Understanding degradation mechanisms: Long-term SOEC testing (1.4 V) and post-mortem samples analysis (INL)**

- 3D compositional analysis has been performed on as-received and cycled (SNL)

**Develop a new computational tool to predict microstructure degradation in HTE systems (LLNL)**

- Analyze representative HTE cell layers and interfaces with high precision at SLAC (NREL)
  - Development of secondary phases (XRD)
  - Interdiffusion of elements (XRD, XAS, XRF)
  - Formation of voids (tomography - TXM)
- ALS tomography, microdiffraction, non-ambient diffraction (LBNL)
5. **STCH Supernode**: Develop Atomistic Understanding of Layered Perovskite \( \text{Ba}_4\text{CeMn}_3\text{O}_{12} \) (BCM) and its Polytypes (LLNL, NREL, SNL; 6 Nodes)

**Goal**: Develop a fundamental understanding of how unique electronic structures, induced by Mn-O ligand bond arrangements, influence favorable water-splitting material behavior.

**Impact**: Discover new STCH materials capable of splitting water at high \( \text{H}_2\text{O}:\text{H}_2 \) ratio. Knowledge gained here supports FOA-awarded projects’ goals.

**Objectives**:
- Discover and synthesize model perovskite system
- Develop and exercise **multi-length-scale** observation platforms and methods
- Apply first principles theory to derive atomistic understanding of water splitting activity
5. STCH Supernode Accomplishments: Discovered New Materials, Demonstrated Hydrogen Production, Developed Advanced Characterization

- Discovered **TWO** new water splitting compounds that are structurally identical and compositional variants to Ba$_4$CeMn$_3$O$_{12}$ (BCM).
  - Identical crystallography
  - Different electronic structure and water splitting behavior

- Demonstrated H$_2$ production capacity of new compounds exceeds CeO$_2$ cycled at $T_R = 1350$ °C.

- Developed research tools and validated methodology.
  - In situ hot stage EELS and high-resolution electron microscopy
  - Operando synchrotron X-ray scattering (SLAC)
  - Ab initio theory (defect thermodynamics)

- Generating foundational knowledge to correlate water splitting activity with electronic structure.
**Best Practices in Materials Characterization**

PI: Kathy Ayers, Proton OnSite (LTE)
Co-PIs: Ellen B. Stechel, ASU (STCH); Olga Marina, PNNL (HTE); CX Xiang, Caltech (PEC)
Consultant: Karl Gross

**Goal:** Development of best practices in materials characterization and benchmarking
Critical to accelerate materials discovery and development

**Accomplishments:**
- 2nd Annual AWS community-wide benchmarking workshop (ASU, Oct. 29–30, 2019)
- 36 test protocols drafted and reviewed
- 40 additional protocols in drafting process
- Relevant operational conditions were assessed for each of the water splitting technologies
- Engaged with new projects at March 2020 kickoff meeting and organized breakout meetings
- Quarterly newsletters disseminated to AWS community

**Development of best practices in materials characterization and benchmarking: critical to accelerate materials discovery and development**
Responses to Previous Year Reviewers’ Comments

• As the consortium matures, it may be helpful to establish formal internal mechanisms for self-assessment, deciding future directions, identifying existing barriers, and selecting concrete steps to take to overcome these to maximize the impact of the nodes and ensure adaptability.

Response: We agree. While these activities are not overtly described or the results summarized in the AMR presentation, the HydroGEN Steering Committee along with guidance from DOE does have internal mechanisms in place to self-assess and take action to maximize consortium effectiveness. While the labs do provide input about future directions, defining and implementing is DOE’s purview. An example of how we have done this is developing the Supernode concept. When we developed the Supernode concept, we identified the major barrier(s) for each of the AWS technologies. These barriers are not being addressed by the FOA-awarded projects and can only be tackled by the HydroGEN labs because of labs’ existing expertise and capabilities. Each Supernode involves multi-lab and multi-node collaboration, has high impact goals and outcomes, and has concrete steps to overcome these barriers.

• By managing the materials characterization within the national laboratory complex, HydroGEN helps industrial–academic teams focus on making progress toward their performance and durability targets.

Response: We agree. The EMN approach leverages the world-class materials characterization capabilities within the national laboratory complex and enables scientific progress in a way that would probably not be achieved by a small project working independently. This materials characterization capability and AWS expertise within the national labs also point to the fact that a good role for the national labs would be to validate and benchmark materials.
Responses to Previous Year Reviewers’ Comments

• Within the results presented, the strong collaboration between the project partners and other R&D peers across the community is clear to see. However, it is recommended that a list of achieved publications be presented so that the multi-laboratory collaboration within HydroGEN and with other institutions can be easily identified.

Response: A list of achieved publications (24) and presentations (88) were included in the “Reviewers-Only Slides” section. A list of patents and patent applications were also included in the same section. Furthermore, we are developing a new publications search engine on the [www.h2awsm.org](http://www.h2awsm.org) website to list publications that pulls directly from H2AWSM Zotero library.

• It is difficult to put in perspective to what extent the accomplishments presented have moved each of the four technologies toward meeting the $2/kg goal. Furthermore, it is difficult to put in perspective where each of the four technologies stands relative to meeting the $2/kg goal. While it is not necessarily a weakness, it would be beneficial to understand how the funding is allocated among the four water-splitting technologies, with which of the four technologies the nodes being utilized align, from which technology data is being accessed, etc. This understand would provide a better understanding of how the capabilities, expertise, and R&D for each technology is being utilized.

Response: The funding is equally allocated among the four water splitting technologies. This is indicated by the same number of projects awarded for each technology as each project received a similar amount of funding. The technology-specific posters and the individual project presentations illustrate how the HydroGEN capability nodes, expertise, and R&D are being utilized.
Proposed Future Work

- Core labs will execute HydroGEN lab nodes to enable successful phase 2 and 3 project activities and work with new phase 1 projects
  - Core labs’ interaction with a specific project will end if that project does not achieve its go/no-go decision metric
- Foster growth of phase 2 Supernode work and continue to collaborate and perform integrated research in the five Supernodes to accelerate AWS research
- Work closely with the Benchmarking Team to establish benchmarking, standard protocols, and metrics for the different water-splitting technologies
- Continue to develop a user-friendly, secure, and dynamic HydroGEN Data Hub that accelerates learning and information exchange within the HydroGEN EMN labs, their partners, and other EMN, AE, PEC, and STCH communities
  - Implement advanced data tool infrastructure improvements and capabilities for more open collaboration and contributions across the HydroGEN consortium, including developing additional data harvesting tools that integrate lab data systems with Data Hub services
- Continue to develop a user-friendly, information rich, and relevant HydroGEN website and implement the publication page
- Outreach

Any proposed future work is subject to change based on funding levels
Summary—HydroGEN Consortium: Advanced Water-Splitting Materials (AWSM)

>80 unique, world-class capabilities/expertise:
  - Materials theory/computation
  - Synthesis
  - Characterization and analysis

- 19 projects successfully passed GNG
- 5 Supernodes passed GNG
- 4 NSF DMREF projects completed
- 11 new Round 2 FOA projects started
- 1 MRS TV HydroGEN video
- 2 annual benchmarking workshops
- 36 AWS standard protocols
- Data Hub >36,500 files, 258 users
- Implemented data governance processes

HydroGEN fosters cross-cutting innovation using theory-guided applied materials R&D to advance all emerging water-splitting pathways for hydrogen production
This work was fully supported by the U.S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy (EERE), Hydrogen and Fuel Cell Technologies Office (HFTO).

Ned Stetson  Katie Randolph  David Peterson  James Vickers  Eric Miller
## Acknowledgements

### NREL Team

**Huyen Dinh, Lead Principal Investigators:**

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# Acknowledgements

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<td>Gabriel Ilevbare</td>
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<td>Dan Ginosar</td>
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Technical Backup Slides
2017 FOA Projects:

1. **Proton Onsite** - High Efficiency PEM Water Electrolysis Enabled by Advanced Catalysts, Membranes and Processes
2. **Argonne National Laboratory** - PGM-free OER Catalysts for PEM Electrolyzer
3. **Los Alamos National Laboratory** - Scalable Elastomeric Membranes for Alkaline Water Electrolysis
4. **Los Alamos National Laboratory** - High-Performance Ultralow-Cost Non-Precious Metal Catalyst System for AEM Electrolyzer
5. **Northeastern University** - Developing Novel Platinum Group Metal-Free Catalysts for Alkaline Hydrogen and Oxygen Evolution Reactions

2019 FOA Projects:

1. **Georgia Institute of Technology** - Interface and Electrode Engineering for Durable, Low Cost Alkaline Anion Exchange Membrane Electrolyzers
2. **The Chemours Company FC, LLC** - Performance and Durability Investigation of Thin, Low Crossover Proton Exchange Membranes for Water Electrolyzers
3. **University of Oregon** - Pure Hydrogen Production through Precious-Metal Free Membrane Electrolysis of Dirty Water
HTE Projects

2017 FOA Projects:

1. Saint-Gobain - Development of Durable Materials for Cost Effective Advanced Water Splitting Utilizing All Ceramic Solid Oxide Electrolyzer Stack Technology
2. United Technologies Research Center - Thin Film, Metal-Supported, High Performance, and Durable Proton-Solid Oxide Electrolyzer Cell
3. University of Connecticut - Proton-Conducting Solid Oxide Electrolysis Cells for Large-Scale Hydrogen Production at Intermediate Temperatures
4. West Virginia University - Intermediate Temperature Proton-Conducting Solid Oxide Electrolysis Cells with Improved Performance and Durability
5. Northwestern University - Characterization and Accelerated Life Testing of a New Solid Oxide Electrolysis Cell

2019 FOA Projects:

1. Nexceris, LLC - Advanced Coatings to Enhance the Durability of SOEC Stacks
2. Redox Power Systems, LLC - Scalable High-H₂ Flux, Robust Thin Film Solid Oxide Electrolyzer
2017 FOA Projects:

1. Arizona State University - Mixed Ionic Electronic Conducting Quaternary Perovskites: Materials by Design for STCH H$_2$
2. Colorado School of Mines - Accelerated Discovery of STCH Hydrogen Production Materials via High-Throughput Computational and Experimental Methods
3. Northwestern University - Transformative Materials for High-Efficiency Thermochemical Production of Solar Fuels
4. University of Colorado Boulder - Computationally Accelerated Discovery and Experimental Demonstration of High-Performance Materials for Advanced Solar Thermochemical Hydrogen Production
5. Greenway Energy - High Temperature Reactor Catalyst Material Development for Low Cost and Efficient Solar Driven Sulfur-Based Processes (Hybrid Sulfur)

2019 FOA Projects:

2. University of Florida - A New Paradigm for Materials Discovery and Development for Lower Temperature and Isothermal Thermochemical H2 Production
PEC Projects

2017 FOA Projects:

1. **Stanford University** - Protective Catalyst Systems on **III-V and Si-Based** Semiconductors for Efficient, Durable Photoelectrochemical Water Splitting Devices

2. **Rutgers University** - Best-in-Class **Platinum Group Metal-Free Catalyst Integrated Tandem Junction** PEC Water Splitting Devices

3. **University of Michigan** - Monolithically Integrated **Thin-Film/Si Tandem** Photoelectrodes

4. **University of Hawaii** - Novel **Chalcopyrites** for Advanced Photoelectrochemical Water-Splitting

2019 FOA Projects:

1. **Rice University** - Highly Efficient Solar Water Splitting Using 3D/2D Hydrophobic **Perovskites** with Corrosion Resistant Barriers

2. **University of Toledo** - **Perovskite/Perovskite Tandem** Photoelectrodes for Low-Cost Unassisted Photoelectrochemical Water Splitting

3. **University of California, Irvine** - Development of **Composite Photocatalyst** Materials that are Highly Selective for Solar Hydrogen Production and their Evaluation in Z-Scheme Reactor Designs