HydroGEN Overview: A Consortium on Advanced Water-Splitting Materials

Huyen N. Dinh (Primary Contact, National Renewable Energy Laboratory [NREL]), Richard Boardman (Idaho National Laboratory [INL], Anthony McDaniel (Sandia National Laboratories [SNL]), Elise Fox (Savannah River National Laboratory [SRNL]), Tadashi Ogitsu (Lawrence Livermore National Laboratory [LLNL], Adam Weber (Lawrence Berkeley National Laboratory [LBNL])
National Renewable Energy Laboratory (NREL)
15013 Denver West Parkway
Golden, CO 80401
Phone: 303-275-3605
Email: Huyen.Dinh@nrel.gov

DOE Manager: Katie Randolph
Phone: 720-356-1759
Email: Katie.Randolph@ee.doe.gov

Project Start Date: June 2016
Project End Date: Project continuation and direction determined annually by DOE

Overall Objectives

- Facilitate collaboration between the four water-splitting pathways on common materials challenges and resource needs.
- Socialize and inform the general hydrogen community about the HydroGEN Energy Materials Network (EMN) consortium.
- Identify new and review current resource nodes that are relevant, unique, and available to support HydroGEN.
- Develop the HydroGEN website to make it user friendly, easily searchable by capability node and/or laboratory, and an information-rich resource about HydroGEN activities.
- Develop and facilitate execution of a catalog of standardized technology transfer agreements (TTAs) that can provide rapid access to the labs.
- Develop an accessible, searchable, and secure HydroGEN Data Hub and SharePoint site to support collaborative science.
- Establish cooperative research and development agreements that leverage the node capabilities of HydroGEN.
- Develop benchmarking standards and procedures to ensure consistency in reporting and proving the principles of advanced water-splitting materials (AWSM).
- Enable funding opportunity announcement (FOA) projects to meet their technical goals through joint research activities and interactions with the nodes.

Fiscal Year (FY) 2019 Objectives

- Align scope of work with the relevant seedling projects' Go/No-Go decision points, and the core labs' interaction with a specific seedling project will end if that project does not achieve its Go/No-Go decision metric.
- Continue to develop a user-friendly, secure, and dynamic HydroGEN Data Hub that accelerates learning and information exchange.
- Continue to work closely with the Benchmarking Team to establish benchmarking, standard protocols, and metrics for the different water-splitting technologies.
- Develop Supernode concepts, one in each of the AWSM technologies, where the core labs work collaboratively to demonstrate the power of integrating and utilizing the HydroGEN capabilities and address a specific research gap.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Production section of the Fuel Cell Technologies Office (FCTO) Multi-Year Research, Development, and Demonstration Plan[1]:

---

[1] https://www.energy.gov/eere/fuelcells/downloads/fuel-cell-technologies-office-multi-year-research-development-and-22

- (F) Capital Cost
- (G) System Efficiency
- (K) Manufacturing
- (L) Operations and Maintenance
- (S) High-Temperature Robust Materials
- (T) Coupling Concentrated Solar Energy and Thermochemical Cycles
- (W) Materials and Catalysts Development
- (X) Chemical Reactor Development and Capital Costs
- (AC) Solar Receiver and Reactor Interface Development
- (AE) Materials Efficiency - Bulk and Interface
- (AF) Materials Durability - Bulk and Interface
- (AG) Integrated Device Configurations
- (AH) Reactor Designs
- (AI) Auxiliary Materials
- (AJ) Synthesis and Manufacturing
- (AL) Operations and Maintenance.

Technical Targets

HydroGEN is an EMN consortium that is led by six National Laboratories (NREL, LBNL, SNL, LLNL, INL, SRNL) and fosters cross-cutting materials innovation, using theory-guided applied materials research and development, to advance all emerging water splitting pathways (low-temperature electrolysis [LTE], high-temperature electrolysis [HTE], photoelectrochemical [PEC] and solar thermochemical [STCH], which includes hybridized thermochemical and electrolysis approaches to water splitting) for clean and sustainable hydrogen production that meets the following DOE targets:

- Cost of hydrogen production: \$2/kg H_2
- Efficiency and durability targets that vary for different water splitting pathways.

FY 2019 Accomplishments

- Expanded the highly collaborative HydroGEN consortium, which currently has 11 national labs, seven private companies, 30 universities, and two funding agencies: DOE FCTO and National Science Foundation Designing Materials to Revolutionize and Engineer our Future (NSF DMREF). Added three new node capabilities and updated more than 40 existing nodes to expand relevance based on seedling project needs.
- Supported the seedling projects Phase 1 research activities and milestone outcomes, helping 18 of 19 projects successfully pass the Go/No-Go milestone.
- Incorporated two new HTE projects.
- Initiated five supernode concepts among the core labs and began Phase 1 research.
- Awarded four NSF DMREF projects and have started collaborative research with HydroGEN capability nodes.
- Contributed to high-value products and disseminated them to the R&D community. These include:
    - A community benchmarking workshop
    - Two Materials Research Society symposia
    - 30 published papers
    - 104 presentations
    - One patent
    - Two provisional applications filed
    - One accepted SLAC National Accelerator Laboratory proposal.
- Collaborated with the benchmarking project team by encouraging seedling project and tenured technical authorities to participate in the Fall 2018 Benchmarking Workshop, by helping lead break-out groups at the workshop, and by writing and reviewing the first round of test protocols in all four AWS technologies.
- Maintained the HydroGEN website and developed four “Working with HydroGEN” video testimonials.
- Expanded the HydroGEN Data Hub’s repository, which currently has 210 users, 29,977 data files, 8 public datasets, and 30 secure project spaces.
- Introduced new data tools to the HydroGEN Data Hub for data ingestion, visualization, and analysis, leveraging other EMNs.

- Upgraded the HydroGEN Data Hub software platform to the latest CKAN version (2.8), enabling cross-lab and cross-EMN development of new Data Hub capabilities, and enabled the capture and reporting of Data Hub usage statistics through an interactive Google Analytics report.
- Extracted, compiled, and uploaded key experimental data from the [former] Nuclear Hydrogen Initiative Program technical progress reports to the HydroGEN Data Hub.

INTRODUCTION

HydroGEN, established in June 2016, is a DOE EMN consortium aiming to accelerate the research, development, and deployment of AWS technologies for clean, sustainable hydrogen production, with a specific focus on materials innovations that lower cost and increase durability. Now in its third year, HydroGEN has become a national innovation ecosystem, producing many high-value products and disseminating them to the R&D community. The consortium's focus is on four promising water splitting pathways: LTE, HTE, STCH, and PEC.

The HydroGEN laboratory resource network comprises 6 core national laboratories: NREL, SNL, LBNL, LLNL, INL, and SRNL due to their emerging capabilities in advanced LTE, HTE, PEC, STCH, and hybridized thermochemical and electrolysis approaches. NREL is the lead lab of the HydroGEN consortium and is tasked with engaging external stakeholders (other labs, universities, and companies), coordinating the development of short-form agreements for engagement with the consortium (e.g., intellectual property agreements and cooperative research and development agreements), and building and managing the launch of an online database that captures relevant data in a user-friendly format. At the end of FY 2019, HydroGEN comprises participants from 11 national labs, seven companies, 30 universities, and two funding agencies— DOE FCTO and NSF DMREF (Figure 1).

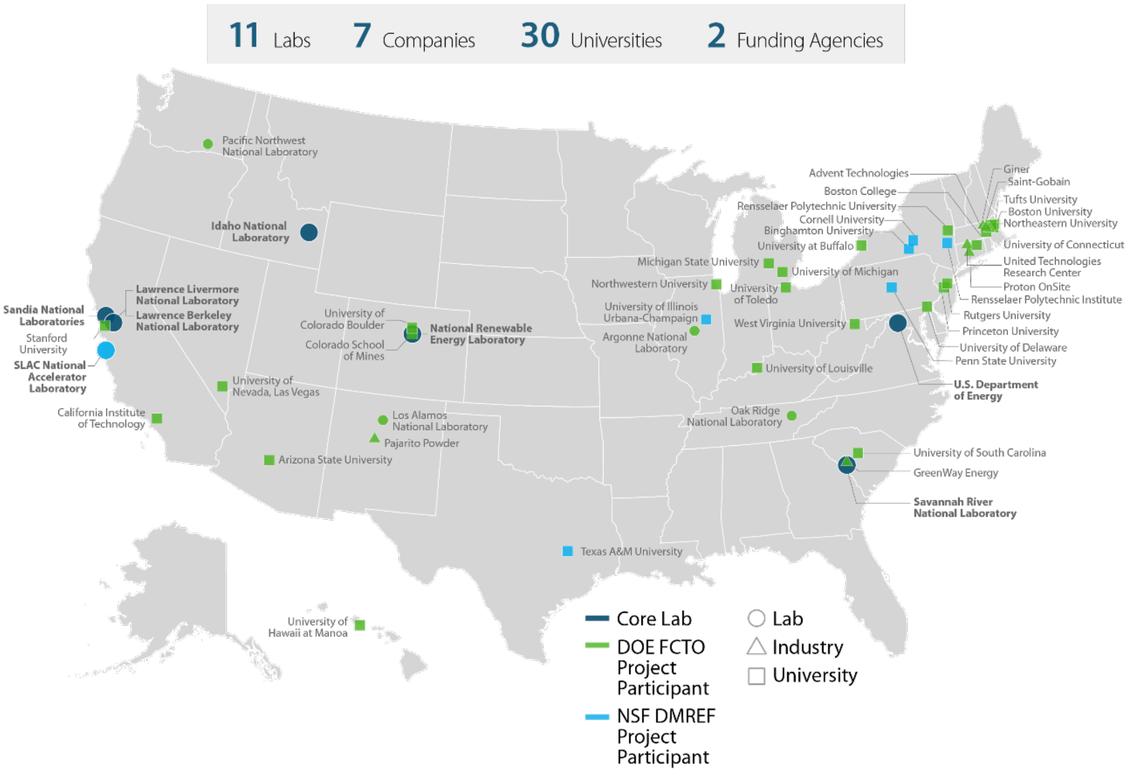

Figure 1. HydroGEN EMN is a nationwide, inter-agency, collaborative consortium focused on early-stage AWS materials R&D for low cost, sustainable hydrogen production.

HydroGEN has a world-class materials capability network, comprising more than 80 unique capabilities/expertise in materials theory/computation, advanced materials synthesis, characterization, analysis, and integration. Each capability represents a resource node—a combination of a tool, technique, and expertise—that is unique to the national laboratory system, available to external stakeholders, and relevant to one of the HydroGEN water-splitting pathways. HydroGEN capability nodes are assigned a readiness category (1, 2, or 3) to inform potential users of their development status. For example, a Category 1 node is fully developed and has been used for AWSM research, while a Category 3 node requires significant development for use by the project partner.

A website for HydroGEN (https://www.h2awsm.org/) provides searchable links to the nodes. The user-friendly node search engine (https://www.h2awsm.org/capabilities) allows stakeholders to quickly identify capability nodes that can be used to advance their materials R&D. Filters allow the nodes to be sorted and queried by water splitting technology, node readiness category, capability class, and national laboratory**.**

APPROACH

The goal of the consortium is to advance the maturity level of the various water-splitting pathways for hydrogen production by offering national laboratory capabilities, including leading technology experts and equipment resources relevant to materials research in these pathways, to outside stakeholders. The consortium addresses the cross-cutting material challenges using a theory-guided, applied materials R&D approach to synthesize and characterize materials that are tested, analyzed, evaluated, and reported through scholarly articles and data bases that are developed and maintained by members of the core labs. While it is recognized that each pathway has unique material and/or integration challenges, one of the strategies of this consortium is to apply these crosscutting core capabilities and expert knowledge across research disciplines and water splitting technology pathways in order to develop critical materials and amplify the consortium's effectiveness.

The consortium performs node capability development that is consistent with the needs of the HydroGEN EMN. The nodes are routinely reviewed and updated to meet the needs of technology developers.

The consortium also supports a benchmarking project team and data team under this EMN to provide a system for data quality control and usefulness for the purposes of achieving the DOE FCTO hydrogen production targets. Benchmarking standards and testing approaches provide a consistent structure by which materials research is standardized across the university and private institutions. This helps (1) accelerate an understanding of the governing principles and phenomena relating to materials properties, functionality and ultimate performance under complex, multi-physical domains, length scales, and time scales; (2) develop uniform analytical and experimental procedures; (3) establish correct experimental parameters that are needed to formulate models that can be used to project materials property microstructure evolution.

The data team leads the development and implementation of a useful Data Hub that serves as a repository for the data and outcomes of the projects supported under HydroGEN. Individuals are welcome to register and explore the Data Hub. HydroGEN project investigators and node leads are authorized to upload and archive the project data in a timely manner. Access to the data is dependent on proprietary conditions but generally is available to associates collaborating on a project. The data team develops web-based tools that help manage the data using state-of-the-art tools to assist experimentalists in storing, retrieving, viewing, and comparing large data sets.

Finally, the consortium is devoted to technology transfer through the DOE process. Each of the core labs follow guidelines and TTA templates, developed to streamline access to the national labs' materials capability network. These standard, pre-approved, mutual TTAs include non-disclosure agreements (NDAs), material transfer agreements, and cooperative research and development agreements (CRADAs)with industry partners (https://www.h2awsm.org/working-with-hydrogen).

RESULTS

HydroGEN FY 2019 R&D Highlights

The HydroGEN EMN has a balanced AWSM R&D portfolio across the six core labs, 21 FOA-awarded materials projects, and one benchmarking project. Of the 80 capability nodes within HydroGEN, more than 49 are being leveraged by the FOA-awarded projects. The HydroGEN core labs performed and supported computational, experimental, and analytical tasks, in collaboration with the FOA-awarded projects. Improvements in efficiency, durability, and/or material cost were achieved in at least five AWSM projects, providing a pathway to meet the hydrogen production cost goal of <\$2/kg-H_2.

More than 40 capabilities were updated this year and three new capability nodes were added to HydroGEN. Under the FY 2019 FCTO H2@Scale FOA, eleven new project awards were announced, raising the total possible DOE-funded AWSM projects accessing the capability nodes to 32. Capability use by other DOE programs, CRADA partners, and strategic partnership projects is also on the rise. Finally, the six core labs are integrating multiple nodes at multiple labs and collaboratively working on specific technology materials R&D topics that can help accelerate the AWSM R&D for the entire AWSM scientific community.

Milestone status for FY 2019

The HydroGEN FY 2019 goal was to identify at least five AWS material systems, through early-stage computational and experimental R&D, that enable pathways to meet the hydrogen production cost goal (through demonstrated improvements in efficiency, durability, and/or cost). This milestone was achieved, and project R&D highlights are reported in the FY 2019 annual reports for each of the HydroGEN seedling projects.

Supernode Development and Outcomes for FY 2019

A new objective in FY 2019 was to establish five supernodes, where the core labs work collaboratively to address a specific and critical research gap and demonstrate the power of integrating and utilizing the HydroGEN capabilities. The following highlights describe some of the accomplishments:

1. **The STCH supernode discovered two new materials for thermochemical water splitting by substitutional modification of the Ba-(Metal)-MnO_x backbone in $Ba_4CeMn_3O_{12}$ (BCM)**. Complete replacement of Ce in BCM produced an equivalent crystallographic structure as BCM, capable of splitting water with greater hydrogen capacity than state-of-the-art CeO_2 (when cycled at low reduction temperature). Another variant formulated by replacing Ce with a different rare earth metal also splits water while maintaining structural similarity to BCM. While water splitting functionality was discovered, which is rare in and of itself, the oxidation behavior of these two new materials is significantly different than BCM and different from one another. Probing the observed differences in chemical redox activity for similar crystallographic structures, that also maintain similar Mn-O coordination, will shed light on how best to engineer next-generation STCH materials.
2. **The Oxygen Evolution Reaction (OER) Modeling supernode has formalized a methodology to go from ab-initio density functional theory (DFT) simulations (NREL) to explicit solvent simulations (LLNL) to microkinetics to macroscale simulations (LBNL).** This work has been utilized to predict surface coverages and reaction mechanisms at pH 0 and pH 1, where the mechanism kinetic barriers come from DFT and the thermodynamic step levels from the more detailed simulations containing solvent. The predicted performance was compared to an experimental rotating disk electrode (RDE) results with a qualitative agreement. Work is ongoing to refine mechanisms, barriers, and experimental data across the pH scale to enable better quantitative agreement and examine the dominant pathways at surface species, the latter of which will be validated by comparison with ambient-pressure XPS measurements. This supernode's goal is to understand and address knowledge gaps about OER across pH ranges through multiscale, multi-theory modeling.
3. **The LTE/Hybrid supernode, comprising three national labs and eight nodes**, **quantified the relationship between ex-situ RDE and in situ membrane electrode assembly (MEA) performance and found that the trends were similar.** This milestone was achieved by evaluating various ionomer compositions and catalyst loadings using rutile iridium (Ir) oxide OER catalyst in RDE and MEA testing. Although similar trends were observed in ex-situ and in-situ testing, ionomer amounts were generally much higher in MEAs. This gap speaks to the differences between liquid and

polymer electrolytes used in the two tests, where the ionomer is needed for proton transport in MEAs, and ionomers only act to disperse inks in RDEs. The goal of this supernode is to integrate ex-situ and in-situ performance, and improve material-specific component to achieve optimized electrolyzer cell performance and durability.

4. **The photoelectrochemical (PEC) supernode has demonstrated scale-up of a photoreactor module to an 8 cm^2 III-V absorber area and evaluated the device on sun for 2+ days while employing in situ current-voltage and impedance measurements and analysis of the electrolyte for corrosion products.** To do so, NREL developed growth of tandem III-V absorber structures on a newer reactor capable of growing on 2-inch diameter substrates. The III-V devices were integrated into an LBNL photoreactor chassis, and baseline characterizations and comparisons were performed in lab and on sun at both NREL and LBNL. The 8 cm^2 device was stable during on sun testing over 3 days with a solar-to-hydrogen-efficiency of 9.2% even after traveling 1,191 miles between LBNL and NREL. This supernode's goal is to understand integration issues and emergent degradation mechanisms of PEC devices at a relevant scale and demonstrate an integrated 50 cm^2 PEC panel.
5. **Under the HTE supernode, five national labs and seven nodes (Figure 2) collaborated to synthesize, characterize, and test the performance of 4–6 model electrode/electrolyte half-cells that have microstructures similar to the pure phase materials**. Microscopy and X-ray diffraction (XRD) analysis confirmed the repeatability of the electrode/electrolyte microstructure and composition. The goal was to synthesize materials that do not have secondary phases, and that the microstructure porosity and pore size are within 10% of each other. This will enable study and understanding of the microstructure evolution phenomenon that causes solid oxide electrolysis cell degradation.

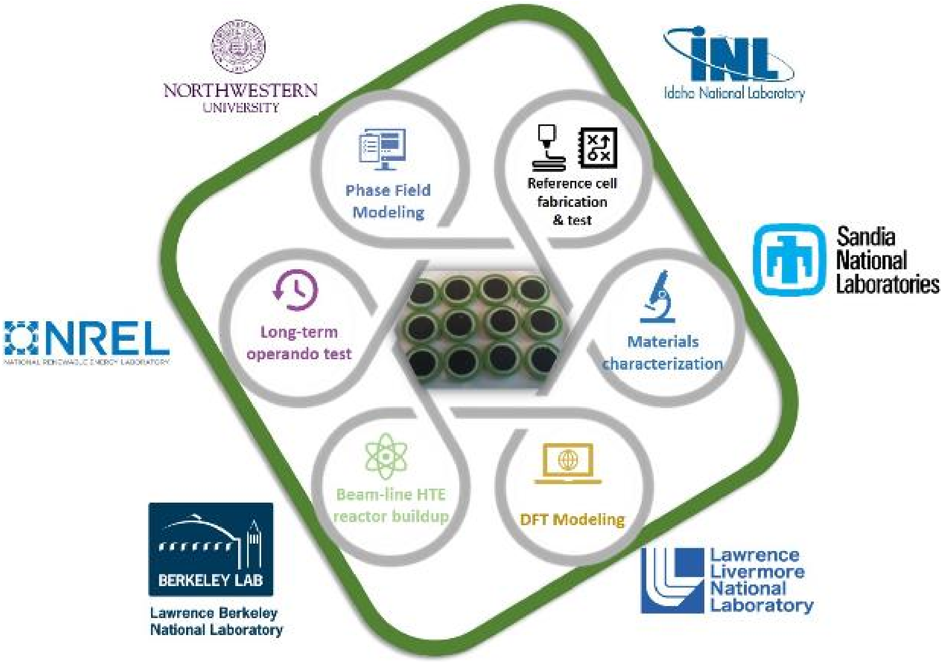

Figure 2. The HTE Supernode is designed to understand HTE electrode microstructure evolution as a function of local solid oxide composition and operating conditions.

HydroGEN FY 2019 Data Team Accomplishment Highlights

NREL led the data team to expand the HydroGEN Data Hub's repository. By the end of FY 2019, the Data Hub had over 210 users, 29,977 data files, and eight public datasets (including AWS technology questionnaires and result summaries, summaries of HydroGEN benchmarking workshop break-out groups, and density functional theory modeling data of BCM STCH materials) (https://datahub.h2awsm.org/dataset). Thirty secure project spaces (including the four NSF DMREF projects) had been established for team members to share data.

In FY 2019, the HydroGEN Data Hub software platform was upgraded to enable the capturing and reporting of Data Hub usage statistics. The open-source codebase for the Data Hub was updated to the latest CKAN version (2.8), providing improved functionality as well as the ability to share the Data Hub instance with other developers—enabling cross-lab and cross-EMN development of new Data Hub capabilities. An interactive Google Analytics report (https://datastudio.google.com/u/0/reporting/1vg8D6JgOjw906hTuym175voJDO9LJ0Ax/page/NjKo) was developed to capture statistics on usage, such as the Data Hub user demographics and geography, as well as popular downloads.

NREL, LBNL, and SNL worked together to develop new capabilities for the HydroGEN Data Hub, including Data Hub Developer capabilities to enable developers to create their own data hub instances for developing new tools and functionality; Dataset Versioning capability to easily track between multiple analysis versions of datasets; Metadata Tools that provide a variety of tools to enable enhanced data upload/download and metadata extraction; and STCH Book to perform automated data management and analysis for STCH data using non-proprietary shared software modules.

The HydroGEN data team implemented data tools for EMN collaboration to perform data exchange and exploration and data visualization and analysis. The following tools were developed in FY 2019:

- Dynamic metadata tool
- Multi-spectra viz tool
- CSV tool
- Polarization curve visualization
- STCH SFR tool (external tool)
- Data processing and upload tool (external tool)
- Multi-file data upload tool for image formats and large numbers of files (external tool, leveraged from ChemCatBio)
- XRD Unimix Analysis tool (external tool, leveraged from ElectroCAT)
- Sample Tracker (external tool, leveraged from ChemCatBio).

When a user uploads many spectra-formatted files (x vs y spectrum), the multi-spectra data tool allows the users to see all the spectra in one single plot.

The multi-file data upload tool automates the extraction of metadata for several different experimental data types (such as microscopy images) and enables researchers to upload many files at once into the Data Hub. For example, it inspects the raw microscopy images and extracts metadata automatically, which are then applied to the files when uploading to the Data Hub. It allows imaging results to be uploaded “en masse” to the data hub.

The XRD Unmix Analysis tool automates the analysis of XRD patterns as compared to reference materials. It uses machine learning to compare a set of experimental XRD results to a chosen reference set and displays the amount of each reference component present in each of the experimental data.

The polarization data visualization tool makes it possible to interactively query and plot results contained in the database. This method of organically linking data and their graphical representation helps relate performance phenomena to materials properties (Figure 3).

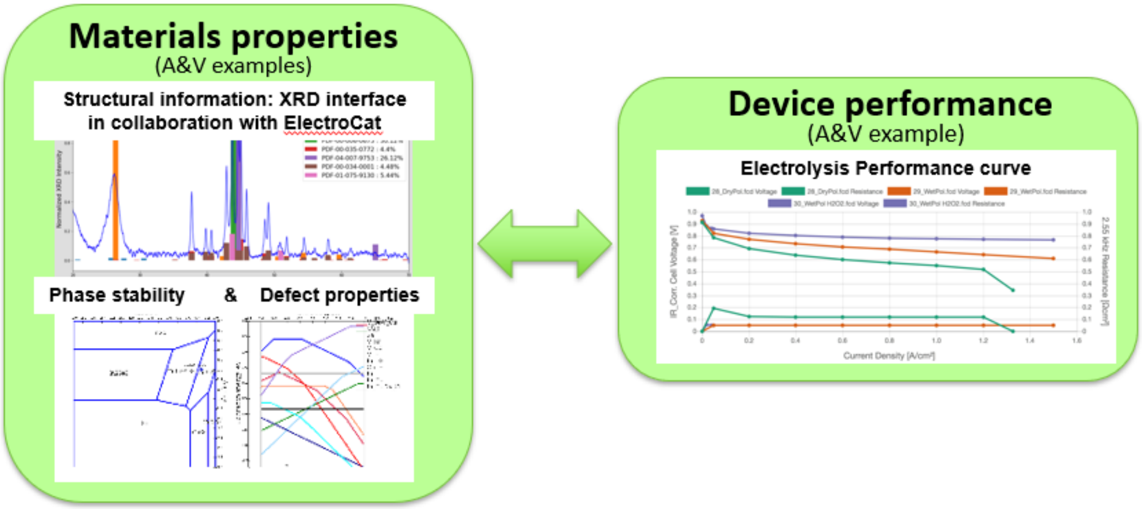

Figure 3. Example of data tools for data ingestion, visualization, and analysis

As a value-add task to the HydroGEN EMN, INL extracted, compiled, and uploaded key computational and experimental data from the [former] Nuclear Hydrogen Initiative Program technical progress reports to the HydroGEN Data Hub. These data from over 20 DOE progress reports published from 2005 to 2012 will next be mapped using metadata so they can be queried using the HydroGEN Data Hub tools. This will give HTE seedling projects the advantage of comparing current outcomes with the historical materials developed by prior research institutions. The combined data will help support modeling efforts of the HTE Supernode.

Benchmarking Activities FY19 Support

HydroGEN EMN lab members collaborated and engaged extensively with the benchmarking team (FOA-awarded project) to organize, participate, and present at the first AWSM Benchmarking Workshop on Oct. 24–25, 2018 at Arizona State University, in Tempe, Arizona. The workshop brought together the national and international water splitting experts to develop material protocols and identify critical parameters. The HydroGEN lab experts were highly involved in writing and reviewing test protocols for each of the AWS technologies, based on those prioritized during the benchmarking workshop. Each technology also included a protocol for establishing common definitions and notations. The development of best practices in materials characterization and benchmarking is critical to accelerate AWSM discovery and development.

CONCLUSIONS AND UPCOMING ACTIVITIES

Conclusions:

- The HydroGEN EMN is a national lab-led consortium comprising six core labs and has expanded to include 31 FOA-awarded materials projects with a balanced AWSM R&D portfolio, one benchmarking project, four NSF DMREF projects, and five national lab-led collaborative Supernode projects
- The HydroGEN core labs performed and supported computational, experimental, and analytical tasks, in collaboration with 18 FOA-awarded projects (awarded in FY 2017), to accelerate AWSM development with improvements in efficiency, durability, and/or material-cost, providing a pathway to meet the hydrogen production cost goal of <\$2/kg-H_2
- Through five Supernodes, the national labs-led collaborative projects targeting critical research gaps in LTE, PEC, HTE, and STCH technologies
- The data team developed a secured HydroGEN Data Hub (https://datahub.h2awsm.org/) for all projects to store, view, and share data with each other and to make digital data accessible to the scientific community and public. The data team has developed, shared, and demonstrated new data tools

- The HydroGEN TTA team developed multiple standard, pre-approved, mutual TTAs, including NDAs, material transfer agreements, intellectual property management plans, and cooperative research and development agreements, to streamline access to the national labs' materials capability network (https://www.h2awsm.org/working-with-hydrogen).

Proposed Future Work:

- Core labs will continue to align the scope of work with the relevant seedling projects' Go/No-Go decision points
- Support the R&D needs of the 11 new seedling projects awarded in FY 2019
- Integrate the whole system (capability nodes, FOA awardees, data infrastructure, TTA) to accelerate the R&D of HydroGEN critical materials development to deployment.
- Continue to review, maintain, and develop current and identify new relevant HydroGEN capability nodes.
- 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, other EMN, and the electrolysis, PEC, and STCH communities.
- Continue to work closely with the benchmarking team to establish benchmarking, standard protocols, and metrics for the different water-splitting technologies.
- Continue to work on Supernode projects and complete Phase 1 Go/No-Go reviews.
- Continue to conduct outreach via conference presentations and participation, benchmarking workshops, website updates, publications, and generally socializing the HydroGEN EMN concept to the community.

FY 2019 SPECIAL RECOGNITIONS AND AWARDS/PATENTS ISSUED

1. "Reversible Solid oxide Cell Operated with A High-Performing and Durable Anode Material for hydrogen and power generation at intermediate temperatures," Dong Ding, Hanping Ding, Wei Wu, and Chao Jiang. US Patent application (16/560,719)
2. "Electrochemical Cells for Hydrogen Gas Production and Electricity Generation, and Related Structures, Apparatus, Systems, and Methods," Dong Ding, Hanping Ding, Wei Wu, and Chao Jiang. US Provisional (62/751, 969), 2018.
3. E. Fox awarded the Distinguished Service Award from the American Chemical Society Division of Energy & Fuels, August 27, 2019.
4. A. Zakutayev was awarded a BES early career award in BES-MSE Materials Chemistry on "Kinetic Synthesis of Metastable Nitrides."

FY 2019 PUBLICATIONS/PRESENTATIONS

1. K. Ayers, N. Danilovic, R. Ouimet, M. Carmo, B. Pivovar, M. Bornstein. "Perspectives on Low-Temperature Electrolysis and Potential for Renewable Hydrogen at Scale." *Annual Review of Chemical and Biomolecular Engineering* 10.1 (2019): 219 – 239.
2. T. A. Kistler, D. Larson, K. Walczak, P. Agbo, I. D. Sharp, A. Z. Weber, N. Danilovic, "Integrated Membrane-Electrode-Assembly Photoelectrochemical Cell under Various Feed Conditions for Solar Water Splitting." *Journal of The Electrochemical Society* 166.5 (2019): H3020 - H3028.
3. T. J. Smart, T. A. Pham, Y. Ping, and T. Ogitsu, "Optical Absorption Induced by Small Polaron Formation in Transition Metal Oxides: The case of Co_3O_4," *Physical Review Materials* 3, 201401(R) (2019).
4. H. Ding, W. Wu, D. Ding. "Advancement of Proton-Conducting Solid Oxide Fuel Cells and Solid Oxide Electrolysis Cells at Idaho National Laboratory (INL)." *ECS Transactions*. 91 (2019): 1029-1034.

5. R. Wang, G. Y. Lau, D. Ding, T. Zhu, and M. C. Tucker. “Approaches for Co-Sintering Metal-Supported BZCY Proton-Conducting Solid Oxide Cells.” *International Journal of Hydrogen Energy*. 44 (2019): 13768-13776.
6. R. Wang, C. Byrne, M. C. Tucker, "Assessment of Co-Sintering as a Fabrication Approach for Metal-Supported Proton-Conducting Solid Oxide Cells," *Solid State Ionics*, 332 (2019): 25-33.
7. W. Wu, H. Ding, Y. Zhang, Y. Ding, P. Katiyar, P. Majumdar, T. He, D. Ding. “3D Self-Architectured Steam Electrode Enabled Efficient and Durable Hydrogen Production in A Proton Conducting Solid Oxide Electrolysis Cell at Temperatures Lower than 600ºC*,” Advanced Science,* 11 (2018): 1870166. Frontispiece Feature: https://onlinelibrary.wiley.com/doi/10.1002/advs.201870070
8. R. Wang, E. Dogdibegovic, G. Y. Lau, M. C. Tucker, "Metal-Supported Solid Oxide Electrolysis Cell with Significantly Enhanced Catalysis." *Energy Technology* 7.5 (2019): 1801154.

Presentations:

1. H.N. Dinh, A.H. McDaniel, A.Z. Weber, R. Boardman, T. Ogitsu, and H. Colon-Mercado, “HydroGEN: A Consortium on Advanced Water Splitting Materials,” Invited presentation, HydroGEN AWS Technology Pathways Benchmarking & Protocols Workshop, Arizona State University, Tempe, AZ (October 24, 2018).
2. H.N. Dinh, “FCTO’s HydroGEN AWSM Energy Materials Network Overview Webinar,” *Invited* presentation, DOE Fuel Cell Technologies Office Webinar (February 7, 2019).
3. H.N. Dinh, K. Randolph, A.Z. Weber, A.H. McDaniel, R. Boardman, T. Ogitsu, D.L. Anton, D. Peterson, and E.L. Miller, “HydroGEN Overview, Projects, and the AWSM Node Capabilities,” *Invited* presentation, Symposium ES11–Advanced Low Temperature Water Splitting for Renewable HydroGEN Production via Electrochemical and Photoelectrochemical Processes, Spring MRS Meeting, Phoenix, AZ (April 24, 2019).
4. H.N. Dinh, D. Anton, R. Boardman, A. McDaniel, T. Ogitsu, A. Weber, “HydroGEN Overview: A Consortium on Advanced Water Splitting Materials,” 2019 DOE Annual Merit Review (April 30, 2019).
5. H.N. Dinh, D. Peterson, K. Randolph, A. Z. Weber, A.H. McDaniel, R. Boardman, T. Ogitsu, and D.L. Anton, “HydroGEN Overview and AWSM Electrolysis Project Updates,” *Invited* presentation, 235th ECS Meeting, Dallas, TX (May 24, 2019).
6. H.N. Dinh, “HydroGEN and H2@Scale: From Materials R&D to Large Scale H_2 Production,” *Invited* presentation, ACI U.S. Hydrogen & Fuel Cells Energy Summit, Boston, MA (July 10–11, 2019).
7. H.N. Dinh, “H2@Scale Energy System and HydroGEN AWSM,” *Invited* presentation, CREATE ME2 Workshop, University of Calgary, Calgary, Alberta, Canada (August 29, 2019).
8. G. Bender, M. Carmo, S. Fischer, T. Lickert, T. Smolinka, and J. Young, “IEA Annex 30 Overview,” *Invited* talk at Proton 2B Workshop: HydroGEN Benchmarking & Protocols Workshop, Tempe, AZ (October 24, 2018).
9. G. Bender, H.N. Dinh, N. Danilovic, and A. Weber, “HydroGEN: Low-Temperature Electrolysis,” Hydrogen and Fuel Cells Program 2018 AMR, Washington, DC (June 13, 2018).
10. J.L. Young, F. Ganci, S. Madachy, S. Fischer, M. Carmo, and G. Bender, “PEM Electrolyzer Characterization and Limitations When Using Carbon-Based Hardware and Material Sets,” 235th ECS Meeting, Dallas, TX (May 26-31, 2019).
11. G. Bender, S. Alia, M. Ulsh, S. Mauger, B. Pivovar, H. Dinh, A. Weber, N. Danilovic, A. Kusoglu, and H. Colon-Mercado, “HydroGEN Supernode—Linking Low Temperature Electrolysis (LTE)/Hybrid Materials to Electrode Properties to Performance,” Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).

12. Jie Zhou, Hans Johansen, Nemanja Danilovic, V. Zenyuk and Adam Z. Weber, "Multiscale Modeling of Multiphase Transport in PEM Water Electrolyzer", 235th ECS, Dallas, TX, May 29, 2019.
13. A. Weber, N. Danilovic, T. Kistler, S. Alia, P. Agbo, "Benchmarking Water-Splitting Materials at the Intersection of Electrocatalysis and Photoelectrochemistry (*Invited*)", MRS Conference, Phoenix, AZ, April 24, 2019.
14. T. Ogitsu, B. Wood, T.A. Pham, A. Weber, N. Danilovic, L.C Weng, E.J. Crumlin, D. Prendergast, S. Alia, R Larsen, and M.A. Ha, "HydroGEN Supernode: Understanding OER Across pH Ranges Through Multiscale, Multi-Theory Modeling," Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).
15. J. Young, H. Doescher, J. Geisz, J. Turner, and T. Deutsch, "Solar-to-Hydrogen Efficiency—Shining Light on Photoelectrochemical Device Performance," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).
16. T. Deutsch, J. Young, C. Aldridge, C. Barraugh, and M. Steiner, "Photoelectrochemical Water Splitting Durability Testing—What Can Half-Cell Results Can Tell Us About Full-Cell Performance?" Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).
17. H. Lim, J. Young, J. Geisz, D. Friedman, T. Deutsch, and J. Yoon, "Surface-Tailored $GaInP_2$ Photocathodes for High Performance Solar Water Splitting," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).
18. J. Young, N. Danilovic, M. Steiner, F.M. Toma, G. Saur, J. Vidal, H. Breunig, D. Friedman, A. Weber, and T. Deutsch, "HydroGEN PEC Supernode—Emergent Degradation Mechanisms with Integration and Scale Up of PEC Devices," Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).
19. Imran S. Khan, Chris Muzzillo, Craig Perkins, Nicolas Gaillard, and Andriy Zakutayev, "$Zn_{1-x}Mg_xO$ contact layer integration with wide band gap $CuGa_3Se_5$ absorbers," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).
20. Khan, K. Heinselman, C. Muzzillo, J. Young, T. Deutsch, A. Zakutayev, and N. Gaillard, "CuGa3Se5/Zn1-xMgxO Photocathodes for Photoelectrochemical Water Splitting," Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).T. A. Pham, T. Smart, Y. Ping, and T. Ogitsu, "Electronic Properties of the Co_3O_4Photoelectrode: Predictions from First-Principles Calculations," 235th ECS Meeting, Dallas, TX (May 26-30).
21. T. A. Pham, Z. Mi, and T. Ogitsu, "Probing the Surface Chemistry and Stability of III-V Photoelectrodes with First-Principles Simulations and In Situ Experiments," 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22-26, 2019).
22. T. A. Pham, "Aqueous Interfaces from Ab-initio Simulations," invited talk at Water: Grand Challenges for Molecular Science and Engineering, Telluride, CO (July 8-13, 2019).
23. B. C. Wood, "Computational hydrogen materials research at the U.S. Department of Energy," invited seminar at Korea Institute of Science and Technology, Seoul, Korea (May 2019).
24. B. C. Wood, "Probing complex interfaces for renewable production and storage of hydrogen," invited seminar at San Francisco State University (February 2019).
25. B. C. Wood, "Hydrogen materials research at the U.S. Department of Energy: A high-performance computing perspective," invited seminar at Hyundai Motors Hydrogen Energy Development Team, Seoul, Korea (October 2018).
26. B. C. Wood, "First-principles discovery and understanding of materials for renewable hydrogen production," invited talk at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, (April 22-16, 2019).

27. B. C. Wood, "Exploring polarization and double-layer effects at electrochemical interfaces within the Effective Screening Medium method," invited talk at American Chemical Society Spring Meeting, Orlando, FL (April 2019).
28. B. C. Wood, "Integrating simulations and experiments to probe complex photoelectrochemical interfaces under realistic operating conditions," invited talk at American Chemical Society Spring Meeting, Orlando, FL (April 2019).
29. J. B. Varley, A. Sharan, T. Ogitsu, A. Janotti, A. D. DeAngelis, and N. Gaillard, "First-Principles Simulations of Stability, Optical and Electronic Properties of Competing Phases in Chalcopyrite-Based Photoelectrodes," 235th ECS Meeting, Dallas, TX (May 26-30, 2019).
30. T. Smart, T. A. Pham, Y. Ping, and T. Ogitsu, "The Nature of Band Gap of Co_3O_4: a Rivisit from First-Principles," American Physical Society March Meeting, Boston, MA (March 4-8, 2019).
31. T. Ogitsu, "Challenges and Opportunities in Multi-Scale Computational Modeling of Photo-electrocatalytic Processes," keynote lecture at 6th International Conference on Physical and Theoretical Chemistry, Zurich, Switzerland (September 2-3, 2019).
32. T. Ogitsu, "Complex Electrochemical Processes Elucidated by Ab-Initio Simulations and In-Situ Characterizations," invited talk at 6th International Conference on Physical and Theoretical Chemistry, Zurich, Switzerland (September 2-3, 2019).
33. S. Lany, "The Electronic Entropy of Charged Defect Formation and Its Impact on Thermochemical Redox Cycles," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).
34. McDaniel, A. Ambrosini, E. Coker, J. Sugar, R. Bell, D. Ginley, S. Lany, P. Parilla, T. Ogitsu, S. Wan, and B. Wood, "Developing an Atomistic Understanding of the Layered Perovskite $Ba_4CeMn_3O_{12}$ and Its Polytypes for Thermochemical Water Splitting—A HydroGEN Supernode," Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).
35. R. Bell, P. Parilla, E. Coker, E. Stechel, and D. Ginley, "Developing Standard Materials for Solar Thermochemical Water Splitting Calibration," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).
36. R. Bell, X. Qian, E. Coker, M. Rodriguez, P. Parilla, S. Haile, and D. Ginley, "In-Situ Defect Mapping of High Temperature STCH Materials in Oxidizing and Reducing Environments," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).
37. R. Bell, D. Ginley, P. Parilla, S. Lany, E. Coker, A. Zakutayev, and A. McDaniel, "Design, Synthesis, and Characterization of High Quality STCH Materials," Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).
38. D. Ding, R. Boardman, J. O'Brien, H. Ding, D. Ginley, H. Dinh, M. Tucker, J. Sugar, B. Wood, S. Barnett, and P. Voorhees, "High Temperature Electrolysis Supernode: Characterization of Solid Oxide Electrode Microstructure Evolution & Advancement of Solid Oxide Proton-Conducting Electrolyzer at Idaho National Laboratory (INL)," Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ (April 22–26, 2019).
39. Ruofan Wang, Conor Byrne, Michael C Tucker, "Proton-Conducting Ceramics for Metal-Supported Solid Oxide Cells", 19th International Conference on Solid State Protonic Conductors, Stowe, VT, Sept 21, 2018.
40. Dong Ding, Wei Wu, Hanping Ding, Ting He. "Development of Proton-Conducting Solid Oxide Electrolysis Cells at Intermediate Temperatures at Idaho National Laboratory. " 234th ECS conference (the American International Meeting on Electrochemistry and Solid State Science, AiMES). Cancun, Mexico, Sept 30-Oct 4, 2018.

41. R. Wang, M. Tucker, "Development of High Performance Metal-Supported Solid Oxide Electrolysis Cells", The Electrochemical Society 234th Meeting (AiMES 2018), Cancun, Mexico, Sept 30-Oct 4, 2018.
42. (invited) Dong Ding. "Development of Electrochemical Processing and Electrocatalysis at intermediate temperatures at Idaho National Laboratory (INL)*."* Lecture for faculty and graduate students. Department of Mechanical and Aerospace, West Virginia University. Morgantown, WV USA, Dec 4, 2018
43. Hanping Ding, Wei Wu, Dong Ding. "A Novel Triple Conducting Electrode for Fast Hydrogen Production in Protonic Ceramic Electrochemical Cells (H-SOECs)*."* 43rd International Conference and Exposition on Advanced Ceramics and Composites (ICACC 2019), Daytona Beach, FL, USA. Jan 27-Feb 1, 2019
44. (invited) Dong Ding. "Advancement of Intermediate Temperature Solid Oxide Energy Conversion Technologies at Idaho National Laboratory." Lecture for faculty and graduate students. Department of Chemical Engineering, University of Louisiana at Lafayette, Lafayette, LA USA, April 1, 2019.
45. Dong Ding, Hanping Ding, Wei Wu. "Advancement of Proton-Conducting Solid Oxide Electrolysis Cells and Fuel Cells at Idaho National Laboratory." 16th International Symposium on Solid Oxide Fuel Cells (SOFC-XVI). Kyoto, Japan. September 8-13, 2019.

Collaborative Meetings Organized and Participated in:

HydroGEN EMN Benchmarking Meetings:

1. HydroGEN Advanced Water Splitting Technology Pathways Benchmarking and Protocols Workshop, organized by E. Stechel, K. Ayers, CX Xiang, and O. Marina, Arizona State University, Tempe, AZ, October 24-25, 2018.

Hydrogen Production Tech Team (HPTT) Review Meetings:

1. HydroGEN Photoelectrochemical Water Splitting Project Reviews, Webinar, February 5, 2019
2. HydroGEN Solar Thermochemical Water Splitting Project Reviews, hosted by A. McDaniel, Sandia National Laboratory, Livermore, CA, June 6, 2019
3. HydroGEN Low Temperature Electrolysis Project Reviews, hosted by Proton Energy Systems, Wallingford, CT, September 18, 2019
4. HydroGEN High Temperature Electrolysis Project Reviews, hosted by, Saint-Gobain, Northborough, MA, September 19, 2019

HydroGEN EMN Organized Conference Symposia:

1. ES11 Symposium: Advanced Low Temperature Water-Splitting for Renewable Hydrogen Production via Electrochemical and Photoelectrochemical Processes, organized by CX Xiang, K. Ayers, T. Deutsch, C. Yan, 2019 Spring MRS, Phoenix, AZ, April 23-26, 2019.
2. ES12 Symposium: Redox-Active Oxides for Creating Renewable and Sustainable Energy Carriers, organized by A. McDaniel, O. Marina, C. Sattler, E. Stechel, 2019 Spring MRS, Phoenix, AZ, April 23-25, 2019.