HydroGEN Overview: A Consortium on Advanced Water-Splitting Materials

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

Overall Objectives

- Facilitate collaboration between the four advanced 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 to ensure that they 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) 2018 Objectives

- Collaborate and conduct research with the new FOA-awarded HydroGEN projects (18 seedling projects and one benchmarking project).
- Facilitate the rapid implementation of non-disclosure agreements (NDAs), material transfer agreements, intellectual property, and contract agreements to streamline access to the labs.
- Review the current palette of lab resource nodes (>80) and identify new resources that can be included in HydroGEN to keep the nodes updated and relevant.
- Enable and enhance the technical accomplishments of FOA projects and achieve project goals through node interactions.
- Further develop the HydroGEN website (e.g., update the capabilities and add publications and presentations).
- Hold workshops with partners focused on each of the four water splitting pathways to increase the collective understanding of R&D activities, needs, node capabilities, and opportunities for collaboration.

Technical Barriers

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

(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 2018 Accomplishments

HydroGEN is an Energy Materials Network (EMN) consortia, comprising >80 unique, world-class 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 at least one of the HydroGEN water-splitting pathways.

- Expanded the highly collaborative HydroGEN consortium, incorporating 19 new FOA-awarded projects working together across four water splitting technologies, and leveraging the six core labs' capabilities and expertise, to accelerate materials research in order to advance the development of water-splitting technologies.
- HydroGEN successfully engaged in an inter-agency collaboration with the National Science Foundation's (NSF) Designing Materials to Revolutionize and Engineer our Future (DMREF) program element, resulting in four NSF DMREF projects that will leverage the HydroGEN EMN experts and capabilities in three water splitting technologies (PEC, LTE, and STCH).
- Produced many high-value products:
    - Collaboration among 11 national labs, 7 companies, and 30 universities
    - Personnel exchanged for collaborative research
    - >100 material samples exchanged
    - >180 registered researchers on the HydroGEN collaboration site

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

  - >25 papers published or submitted for publication
  - Two records of inventions
  - One facility proposal submitted
  - One EMN-wide meeting on Machine Learning and Data Analytics organized.
- Continually updated and expanded the HydroGEN website (https://www.h2awsm.org/). It currently houses 14 news items, and a new publication subsite that compiles lists of HydroGEN journal articles (13) published, and presentations (21) given. The capability nodes have been reviewed and updated on the user-friendly node search engine.
- Eighteen FOA-awarded projects utilized 44 nodes.
- Established 40 new or substantially updated nodes.
- Maintained and expanded the HydroGEN Data Hub (https://datahub.h2awsm.org/), a secure project space for team members to store, view, and share project data and to disseminate data to the scientific community and public once the private, secure data has been reviewed and curated. The Data Hub has 128 users and 3,889 data files. Three Data Hub highlights include:
  - Developed, shared, and demonstrated new data tools for visualization, uploading large datasets, and metadata assignments.
  - Advanced metadata definitions and application program interface (API) access.
  - Established a data publication process.
- 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).
  - The standard HydroGEN NDAs were signed by all six core labs within two months.
  - The 19 new FOA project NDAs were executed within two weeks.

INTRODUCTION

HydroGEN, established in June 2016, is a DOE EMN consortium aiming to accelerate the research, development, and deployment of advanced water-splitting technologies for clean, sustainable hydrogen production, with a specific focus on materials innovations that lower cost and increase durability.

The consortium's focus is on four promising water-splitting pathways:

- Low-temperature electrolysis (LTE)
- High-temperature electrolysis (HTE)
- Solar thermochemical hydrogen production (STCH)
- Photoelectrochemical hydrogen production (PEC).

The HydroGEN laboratory resource network comprises six core national laboratories—NREL, SNL, LBNL, LLNL, INL, and SRNL—due to their core and 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 2018 HydroGEN comprised participants from 11 labs, 7 companies, and 30 universities (Figure 1).

Figure 1. HydroGEN is a national ecosystem where national labs, universities, and industry partners work together on four emerging, early-stage, advanced water-splitting pathways to produce clean, low-cost, and sustainable hydrogen

HydroGEN has a world-class materials capability network, comprising >80 unique, capabilities/expertise in materials theory/computation, advanced materials synthesis, characterization, analysis, and integration (Figure 2). 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. A category 3 node requires significant development for use by an AWSM project partner.

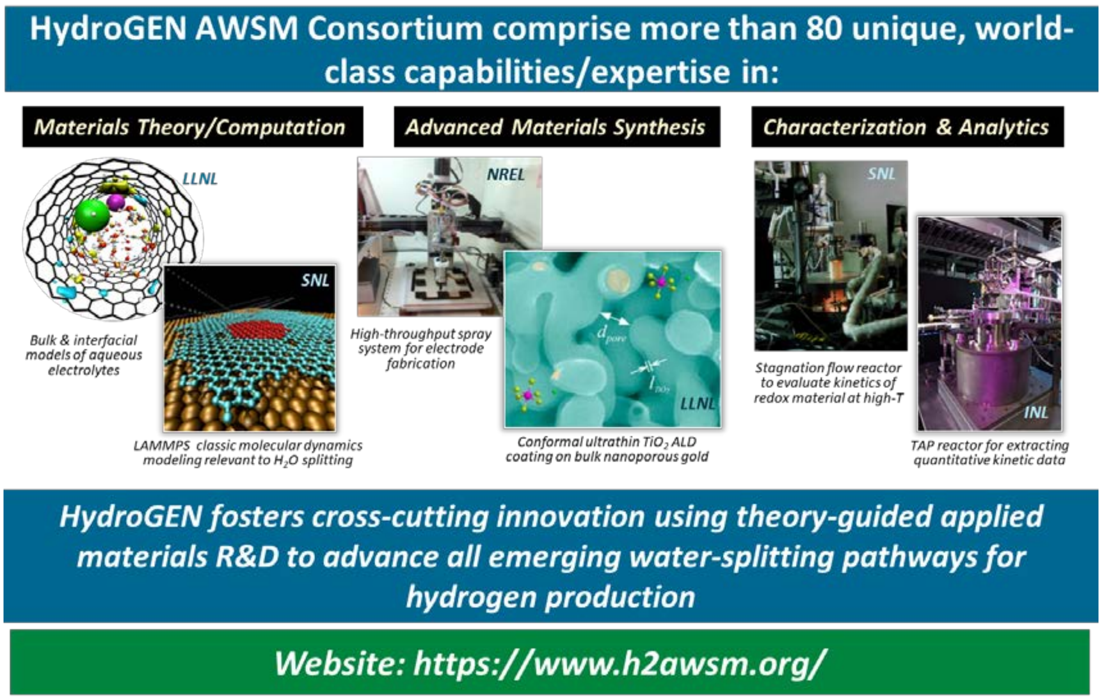

Figure 2. The HydroGEN AWSM consortium fosters cross-cutting innovation using the world-class, unique capabilities and expertise in materials theory and computation, advanced materials synthesis, and characterization at the national labs

APPROACH

The goal of the consortium is to advance the level of maturity 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 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 research and development.

The consortium addresses the cross-cutting material challenges using synthesis and characterization methods that are guided by computational studies and fundamental materials science knowledge. While it is recognized that each pathway has unique material and/or integration challenges, one of the strategies of this consortium is to apply its 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.

RESULTS

The HydroGEN EMN is a large consortium comprising more than 180 individual participants, including technology and capability node experts, principal investigators (PIs), postdoctoral researchers, graduate students, data experts, TTA experts, communications specialists, and website developers. NREL created a user-friendly, secured collaboration (SharePoint) site to enhance communication, information sharing, and collaboration among the 19 FOA-awarded project members, the steering committee members, Fuel Cell Technologies Office leadership team, the Data Team, the TTA team, and the lab node experts. NREL's Data Team has developed a secured Data Hub for all projects to share data with each other. The Data Team, which has representation from the six core national labs, has monthly teleconferences. HydroGEN's steering committee, similarly represented by the six labs, has biweekly webinars to ensure effective communication, timely progress, and transparency.

HydroGEN FY 2018 Data Team Highlights

Developed, shared, and demonstrated new data tools: The Data Team has developed several new data tools for use in the HydroGEN Data Hub, including the Multi-spectra Viz tool for visualizing multiple spectra files together in one graph; the EMN Intelligent Uploader tool written in Python for uploading large datasets of transmission electron microscopy, X-ray diffraction, and Raman spectroscopy with automated metadata; the Defect Properties Viz tool developed by LLNL for dynamic visualization of defect functional properties in allowed composition space; and the stagnation flow reactor (SFR) Data Tool, developed by SNL, for data packaging, metadata assignment, and upload of large experimental datasets from SFR experiments. The Data Team has also implemented "data tool demos" within the User Resources project so that everyone can see example of the data tools and how they work.

Developed advanced metadata definitions and API access: The Data Team continued to refine and develop metadata standards for data types common in HydroGEN. Specifically, the Data Team has made improvements to the data-set-level metadata definitions, as well as individual file-level metadata. The faceted search capability enables quick search across all data sets (across projects as security allows) based on the metadata defined. The Data Team hosted an API tutorial to educate researchers on how to programmatically upload data into the Data Hub as well as write programs to search and download data, based on metadata values.

Established a data publication process: The data publication process enabled making data sets publicly available. This process involves the following steps: PI requests a data set be made public; steering committee reviews; Data Team curates a digital object identifier from the Office of Scientific and Technical Information and assigns it to the data set; and Data Hub administrator moves the data set to public availability. The digital object identifier enables researchers to identify the related data set within the references of publications so that readers can link back to the relevant data.

HydroGEN FY 2018 R&D Highlights

The HydroGEN EMN has a balanced AWSM R&D portfolio (Figure 3) across the six core labs, 18 FOA-awarded materials projects, and one benchmarking project. Of the 80 capability nodes within HydroGEN, more than 44 are being leveraged by the FOA-awarded projects. Furthermore, >35 capabilities have been updated this year and five new capability nodes were added to HydroGEN. The HydroGEN core labs performed and supported computational, experimental, and analytical tasks, in collaboration with 18 FOA-awarded projects, and documented at least three AWSMs with improvements in efficiency, durability, and/or material cost, providing a pathway to meet the ultimate hydrogen production cost target of <\$2/kg H_2. Below are some HydroGEN project R&D highlights for each water-splitting pathway.

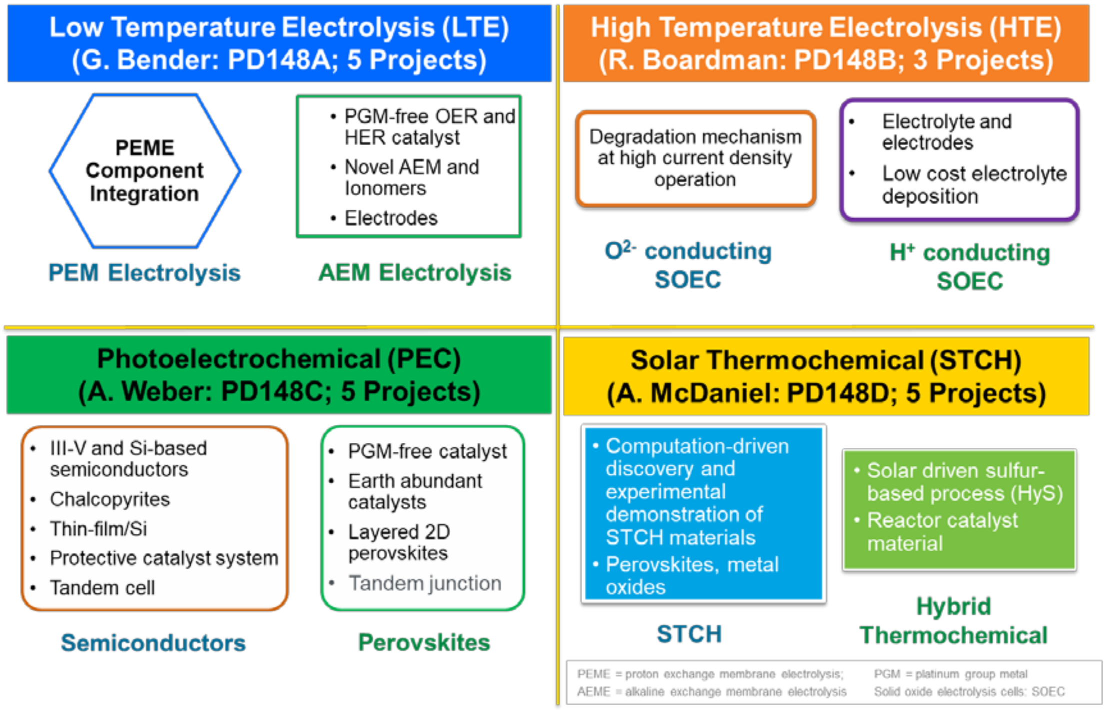

Figure 3. HydroGEN has a balanced AWSM R&D portfolio across the six core labs, 18 FOA-awarded materials projects, and one benchmarking project

PEC:

- Rutgers University, together with the NREL MOVPE III-V semiconductor synthesis and NREL PEC characterization nodes, demonstrated that Rutgers' platinum group metal (PGM)-free Ni_5P_4 hydrogen evolution reaction catalysts/TiN on p-$GaInP_2$ have performance on par with and stability greater than that of PGM catalysts (PtRu/p-$GaInP_2$). When NREL's high-performance photoabsorber ($GaInP_2$/GaAs) was optimized and integrated with Rutgers' PGM-free electrocatalysts ($LiCoO_2$ oxygen evolution reaction and Ni_5P_4 hydrogen evolution reaction catalysts) and protection layer (TiN) for unassisted water splitting, a solar-to-hydrogen efficiency of 11.5% was achieved, which is greater than the go/no-go solar-to-hydrogen efficiency metric of 10%. This was tested and verified by the NREL PEC benchmarking node.

- The performance and corrosion mechanisms of University of Michigan (UM) GaN/Si and T_3N_5 photoelectrodes were characterized and optimized by the NREL "Surface Analysis Cluster Tool," NREL "Surface Modifications for Catalysis and Corrosion Mitigation," and LBNL "Probing and Mitigating Chemical and Photochemical Corrosion of Electrochemical and Photoelectrochemical Assemblies" nodes. The UM project is focused on developing Si-based high-efficiency PEC tandem water-splitting devices, using nanowire tunnel junction to fabricate 1.7–2.0 eV top photoelectrodes on Si wafers and N-terminated GaN to protect against photocorrosion. A GaN/Si photocathode with stable operation for >100 h at a very high photocurrent density of ~38 mA/cm^2, without using any extra surface protection, was demonstrated. Detailed theoretical studies of the GaN surfaces and GaN/water interfaces have also been performed by the LLNL "Computational Materials Diagnostics and Optimization of Photoelectrochemical Devices" node to better understand the effect N-terminated GaN surfaces have on solar water splitting. These studies are further correlated with the stability analysis of the photoelectrodes.

- University of Hawaii, together with the LLNL "Computational Materials Diagnostics and Optimization of Photoelectrochemical Devices" node, investigated the thermodynamic stability of chalcopyrite compounds and competing phases (e.g., ordered vacancy compound) that can form during fabrication and processing of the photoabsorber chalcopyrite materials, and the impact the ordered vacancy compound phase can have on device performance. This understanding can help tune the material synthesis process conditions to achieve the desired ordered vacancy compound-type phases and enhance device performance. The NREL "I-III-VI Compound Semiconductors for Water Splitting" node successfully integrated chalcopyrite on transparent conductive substrate via deliberate alkali doping ($CuGa_3Se_5$ doped with NaF) and achieved the best photocurrent onset (0.4 V vs. reversible hydrogen electrode) ever observed for bare $CuGa_3Se_5$, making it a promising material for tandem water splitting devices.

LTE:

- Proton Onsite met and exceeded near-term performance targets of 1.85 V at 2.0 A/cm^2, using Proton-synthesized high-activity IrRu oxide catalysts of different compositions. Proton's proton exchange membrane water electrolysis cell also demonstrated 800 h of durability at 2 A/cm^2, operating at 80°C and 30 bar. The NREL "Electrolysis Catalyst Ex-situ Characterization and Standardization" node contributed toward a better understanding of IrRu oxide catalyst stability. Proton's improved cell efficiency is a step toward achieving its proton exchange membrane water electrolysis cell efficiency goal of 43 kWh/kg (1.7 V at 90°C) and at a cost of $2/kg H_2, a huge improvement from the state-of-the-art cell efficiency of 53 kWh/kg.

- Collaboratively, LANL, SNL, and NREL demonstrated promising alkaline exchange membrane water electrolysis performance, comparable to iridium oxide, using SNL's anion exchange membrane node, LANL-developed PGM-free oxygen evolution reaction perovskite catalyst, and NREL's expertise in membrane electrode assembly fabrication ("Multicomponent Ink Development, High-Throughput Fabrication, and Scaling Studies" node) and cell electrolysis testing ("In-Situ Testing Capabilities for Hydrogen Generation" node).

- ANL, together with the LLNL "Ab Initio Modeling of Electrochemical Interfaces" and LBNL "Density Functional Theory and Ab Initio Calculations" nodes, investigated the factors that may alter the transport property of a cobalt-based oxygen evolution reaction catalyst, developed by ANL for proton exchange membrane electrolysis. The LLNL team found the origin of the discrepancy between the reported experimental and theory-derived electronic structure of cobalt oxide. This resulted in the confidence to choose a specific theory that can provide reliable information about the electronic structure of the cobalt oxide materials family. This is crucial to reliably identify the factors that determine the transport property of this material, which affects the overall catalytic activity.

HTE:

- Using Northwestern University catalyst, YSZ electrolyte ($(ZrO_2)_{0.92}(Y_2O_3)_{0.08}$), and LBNL "Metal-Supported Solid Oxide Cell" and INL "Advanced Electrode and Solid Electrolyte Materials for Elevated Temperature Water Electrolysis" nodes, the collaboration demonstrated a metal-supported solid oxide electrolysis cell (SOEC) for the first time in electrolysis mode, with the highest performance for oxygen-conducting-type electrolysis cells to date and promising stability. The advantages of a metal-supported SOEC are low cost, high strength, and thermal cycling capability. Furthermore, the data from INL SOEC button cell tests will help Northwestern University establish a deeper understanding of cell degradation, a major barrier for SOECs.

- Three HydroGEN EMN nodes (LBNL, INL, and NREL) provided critical support to the United Technologies Research Center proton-conducting SOEC project by addressing technical barriers in metal alloy durability, electrode/electrolyte material optimization and stability, and SOEC modeling. Various combinations of metal alloys and protective coatings were identified as acceptable for proton-SOEC conditions. High-performance proton electrolytes and steam electrodes were identified and tested by the INL "Advanced Materials for Elevated Temperature Water Electrolysis" node. The resulting button cell performance exceeded the DOE performance target. An electrochemical model and a cell model were developed by the NREL "Multi-Scale Thermochemical and Electrochemical Modeling for Material Scale-Up to Component and System Design" node for SOEC performance characterization and to simulate cell/stack operation for material scale up. In addition, INL provided critical support in cell performance testing for United Technologies Research Center and the University of Connecticut.

STCH:

- Colorado School of Mines, along with NREL's "First Principles Materials Theory for Advanced Water Splitting Pathways" and "Thin Film Combinatorial Capabilities for Advanced Water Splitting Technologies" capability nodes, were able to validate their approach to combine theoretical and experimental materials discovery. First principles theory was used to screen for potential candidates using descriptors developed by NREL that can greatly reduce the search space and associated computational effort. The team envisions building combinatorial libraries of these theory-inspired material formulations and using optical techniques for rapid analysis of redox potential. With the candidate material formulations beginning to emerge from theory, the team produced thin films from materials with known redox behavior in order to develop and validate experimental protocols and further refine their optical analysis methods.

- Arizona State University is developing an all-density-functional-theory methodology for producing CALPHAD model results to more rapidly derive state maps of important thermodynamic relationships in redox materials; namely the dependence of defect concentration on temperature and oxygen partial pressure. SNL's "Uncertainty Quantification in Computational Models of Physical Systems" node is using Bayesian statistical uncertainty quantification to assess the impact of imperfect knowledge (i.e., the synthetic CALPHAD model predictions) on the outcome of computational material screening. Thus far, the computations are able to reproduce experimental redox and water-splitting behavior for CeO_2 and Zr-doped CeO_2, as well as identify sufficiently robust functionals for deriving the aforementioned thermodynamic relationships.

- The University of Colorado Boulder, with help from NREL's "First Principles Materials Theory for Advanced Water Splitting Pathways" node, was able to develop and apply machine learning models to identify ~28,000 stable perovskite formulations (both simple and complex) from over 1.1 million possible candidates. And from this pool of stable perovskites, several hundred materials have oxygen vacancy formation energies in the range of interest for STCH materials. SNL's "Virtually Accessible Laser Heated Stagnation Flow Reactor" and "High-Temperature X-ray Diffraction" nodes are validating the results of the machine-learned thermodynamic screening by characterizing water splitting kinetics and crystal structures for a select number of these material formulations.

Hybrid:

- Greenway Energy (GWE) is developing a hybrid-sulfur system for low-cost and efficient hydrogen production. In collaboration with University of South Carolina, GWE and INL "Catalysts for Harsh Environment" node demonstrated a 30% improvement in performance and better stability for a novel catalyst that can lead to lower hydrogen costs by minimizing or replacing the use of PGM catalysts. An Invention Disclosure Record, listing both University of South Carolina and INL staff, was filed for the composition and synthesis of the catalyst. GWE and NREL "Engineering of Balance of Plant for High-Temperature Systems" node collaboratively designed a balance-of-plant system and developed a novel solar receiver/reactor integrated with the novel NREL solar-plant design that has the potential to eliminate $60 million in cost from a particle-based baseline hybrid-sulfur system and will allow a hydrogen cost reduction of almost 50% compared to the previous baseline economic assessment ($2.5/kg vs. \$5.18/kg H_2). A Record of Invention for the hybrid-sulfur system and the receiver reactor was filed. SRNL "Flow Sheet Development Technoeconomic Analysis" node developed a flow sheet to allow for a direct-solar-heated high-temperature decomposition reactor. Independent operation of the two primary reaction steps with storage of water, liquid SO_2, and concentrated sulfuric acid allowed Greenway Energy to take advantage of fluctuations in cost and availability of electricity. Furthermore, optimal conditions for operation of the high-temperature decomposition reactor were identified. Possibilities for further improvements in efficiency were also identified and should help drive production cost closer to the \$2/kg H_2 target in the next phase.

HydroGEN EMN lab members collaborated and engaged extensively with the Benchmarking Team (FOA-awarded project) to develop four AWSM questionnaires, four AWSM test frameworks, two working group meetings, conference presentations, and >80 HydroGEN capability node assessments. 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 18 FOA-awarded materials projects with a balanced AWSM R&D portfolio, one benchmarking project, and four NSF DMREF collaborative projects.
- The HydroGEN core labs performed and supported computational, experimental, and analytical tasks, in collaboration with 18 FOA-awarded projects, to accelerate the AWSM development with improvements in efficiency, durability, and/or material cost, providing a pathway to meet the ultimate hydrogen production cost target of <\$2/kg H_2.
- 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 for visualization, uploading large datasets, and metadata assignments; advanced metadata definitions and API access; and established a data publication process.
- 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 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.
- 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 among the HydroGEN EMN labs, their partners, other EMNs, and the advanced 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.
- Develop supernode concepts, one in each of the AWSM technologies, through which the core labs work collaboratively to demonstrate the power of integrating and utilizing the HydroGEN capabilities and to address a specific research gap.
- Conduct outreach via conference presentations and participation, benchmarking workshops, website updates, publications, and generally socializing the HydroGEN EMN concept to the community.

SPECIAL RECOGNITIONS AND AWARDS/PATENTS ISSUED

1. "Nanofiber Electrocatalyst," Di-Jia Liu and Lina Chong, US patent application filed in 2018.
2. "Prussian Blue Analogue-Derived Catalysts for PEM Electrolyzer," Di-Jia Liu and Hao Wang, US patent application filed in 2018.
3. Zetian Mi was elected Fellow of Optical Society of America in 2018.

FY 2018 PUBLICATIONS/PRESENTATIONS

Publications

1. Sheng Chu, Srinivas Vanka, Yichen Wang, Jiseok Gim, Yongjie Wang, Yong-Ho Ra, Robert Hovden, Hong Guo, Ishiang Shih, and Zetian Mi. "Solar Water Oxidation by an InGaN Nanowire Photoanode with a Bandgap of 1.7 eV." *ACS Energy Lett*. 3, no. 2 (January 2, 2018): 307–314. https://doi.org/10.1021/acsenergylett.7b01138.
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16. Article in March 2018 issue of *Chemical Engineering* (www.chemengonline.com) titled "Solar Chemistry Heats Up" written by staff editor Gerald Ondrey.
17. Darwin Arifin and Alan W. Weimer. "Kinetics and Mechanism of Solar-thermochemical H_2 and CO Production by Oxidation of Reduced CeO_2." *Solar Energy* 160 (2018): 178–185, doi:10.1016/j.solener.2017.11.075.
18. Harnoor Kaur, Meng Wanga, Maximilian B.Gorensek, and Chau-Chyun Chen. "Thermodynamic modeling of the hybrid sulfur (HyS) cycle for hydrogen production." *Fluid Phase Equilibria* 460 (March 25, 2018): 175–188. https://doi.org/10.1016/j.fluid.2017.12.025.
19. Maximilian B. Gorensek, Claudio Corgnale, and William A. Summers. "Development of the hybrid sulfur cycle for use with concentrated solar heat. I. Conceptual design." *International Journal of Hydrogen Energy* 42 (2017): 20939.
20. Taylor R. Garrick, Cody H. Wilkins, Andrew T. Pingitore, Jacob Mehlhoff, Alex Gulledge, Brian C. Benicewicz, and John W. Weidner. "Characterizing Voltage Losses in an SO_2 Depolarized Electrolyzer Using Sulfonated Polybenzimidazole Membranes." *Journal of the Electrochemical Society* 164 (2017): F1591–F1595.

Presentations

1. (**Invited**) Anthony H. McDaniel and Ivan Ermanoski, "Perovskites and Particle Reactor: A Multinational Effort to Advance Solar Hydrogen," ASME Power Energy 2018 Conference, Orlando, FL, June 2018.
2. Z. Ma, J. Martinek, P. Davenport, and C. Corgnale, "Integrating Thermochemical and Electrochemical Processes with a Concentrating Solar Thermal System for Hydrogen Production," ASME Power Energy 2018 Conference, Orlando, FL, June 2018.
3. (**Invited**) H.N. Dinh, J.W. Vickers, K. Randolph, A.Z., Weber, A.H. McDaniel, R. Boardman, T. Ogitsu, H. Colon-Mercado, D. Peterson, and E.L. Miller, "HydroGEN: An AWSM Energy Materials Network," 233rd Electrochemical Society Meeting, Seattle, WA, May 2018.
4. (**Invited**) K.E. Ayers, "Low Temperature Electrolysis for Hydrogen and Oxygen Generation - a Tutorial on Catalyst and Electrode Development for Proton and Anion Exchange Membrane-Based Systems," 233rd Electrochemical Society Meeting, Seattle, WA, May 2018.

5. (**Invited**) J. Holladay, B. S. Pivovar, K. E. Ayers, O. A. Marina, E. B. Stechel, and C. Xiang, "An Overview of H2@Scale and Water Splitting Protocol Development," 233rd Electrochemical Society Meeting, Seattle, WA, May 14, 2018.
6. (**Invited**) S. Mukerjee, J. Li, and Q. Jia, "Current understanding of the slow kinetics of the hydrogen evolution reaction in alkaline media," 233rd Electrochemical Society Meeting, Seattle, WA, May 13–17, 2018.
7. Q. Jia, J. Li, and S. Mukerjee, "Understanding the improved kinetics of the hydrogen evolution/oxidation reactions of the Pt-oxophilic metal systems in alkaline medium," 233rd Electrochemical Society Meeting, Seattle, WA, May 13–17, 2018.
8. H.T. Chung, A.S. Lee, Y.S. Kim, C. Fujimoto, L.W. Wang, G. Teeter, G. Bender, and P. Zelenay, "Carbon-Free Perovskite Oxide Oxygen Evolution Reaction Catalysts for AEM Electrolyze," 233rd Electrochemical Society Meeting, Seattle, WA, May 2018.
9. Chengxiang ("CX") Xiang, "Development of Best Practices and Standard Protocols in Benchmarking Photoelectrochemical (PEC) Hydrogen Production," 233rd Electrochemical Society Meeting, Seattle, WA, May 17, 2018.
10. S. Hwang, A.B. Laursen, S.H. Porter, Y. Hongbin, M. Li, V. Manichev, K.U.D. Calvinho, V. Amarasinghe, M. Greenblatt, E. Garfunkel, and G.C. Dismukes, "Titanium Nitride As a Conducting Interfacial Layer between Hydrogen Evolution Catalysts and Silicon Photocathodes for Stable Solar-to-Hydrogen Water Splitting Devices," 233rd Electrochemical Society Meeting, Seattle, WA, May 17, 2018.
11. (**Invited**) T. Ogitsu, J. Varley, A.D. DeAngelis, K. Horsley, and N. Gaillard, "Integrating Ab-Initio Simulations and Experimental Characterization Methods: Towards Accelerated Chalcopyrite Materials Development for Hydrogen Production," 233rd Electrochemical Society Meeting, Seattle, WA, May 15, 2018.
12. Boxun Hu, Ashish N. Aphale, Michael Reisert, Seraphim Belko, Olga A. Marina, Jeffry Stevenson, and Prabhakar Singh, "Solid Oxide Electrolysis for Hydrogen Production: From Oxygen Ion to Proton Conducting Cells," 233rd Electrochemical Society Meeting, Seattle, WA, May 13–17, 2018.
13. (**Invited**) Z. Mi, "Artificial Photosynthesis on III-Nitride Nanowire Arrays," 233rd Electrochemical Society Meeting, Seattle, WA, May 13–17, 2018.
14. (**Invited**) Z. Mi, "Solar Water Splitting and CO_2 Reduction on III-Nitride Nanostructures," MRS Spring Meeting, Phoenix, AZ, April 2–6, 2018.
15. (**Invited**) D. Wang, "Understanding the Interface between Photoelectrodes and Catalysts," MRS Spring Meeting, Phoenix, AZ, April 2–6, 2018.
16. H. Hajibabaei and T. Hamann, "Direct Deposition of Crystalline Tantalum Nitride (Ta3N5) on FTO via High-Temperature Atomic Layer Deposition (ALD)," Gordon Research Conference; Renewable Energy: Solar Fuels, January 28–February 2, 2018.
17. (**Invited**) H.N. Dinh, K. Randolph, E. Miller, "An EMN Model for Early R&D," 2018 DOE Hydrogen and Fuel Cell Technical Advisory Committee (HTAC) Meeting, Washington, DC, February 14, 2018.
18. S. Hwang, S.H. Porter, A.B. Laursen, H.Yang, M. Li, V. Manichev, K.U.D. Calvinho, V. Amarasinghe, M. Greenblatt, E. Garfunkel and G.C. Dismukes, "Nickel Phosphide Catalyst and Titanium Nitride Protection Layer for High Efficient and Stable Siliconbased Photocathode," Annual Meeting at Catalysis Society of Metropolitan New York, Lehigh University, April 2018.
19. A. Kashi, S. Hwang, A.B. Laursen, G.C. Dismukes, "Characterization of Highly Active Electrodeposited LixCoO2 Thin Film Anodes in PGM-free Photoelectrochemical Cells," Annual Meeting at Catalysis Society of Metropolitan New York, Lehigh University, April 2018.
20. (**Invited**) Dong Ding, "Application of Intermediate-Temperature Electrochemical Processes in Energy Conversion Technologies at Idaho National Laboratory (INL)," Lecture for faculty and graduate students,

Department of Chemical and Materials Engineering, New Mexico State University, Las Cruces, NM, April 27, 2018.

21. (**Invited**) Anthony McDaniel, Debora R. Barcellos, Michael Sanders, Joshua Sugar, Ryan O'Hayre, "Hydrogen Production by Solar Thermochemical Water Splitting: Searching for Optimal Nonstoichiometric Perovskite Oxides," 255th ACS National Meeting & Exposition, New Orleans, LA, March 2018.
22. Huyen N. Dinh, "An Overview of HydroGEN: A DOE Energy Materials Network, Aimed at Accelerating the R&D of Advanced Water Splitting Materials," Fuel Cell Seminar and Energy Exposition, Long Beach, CA, November 2017.
23. Zhiwen Ma, "Concentrating Solar Power Technology for Green Syngas and Hydrogen Production," 2017 Syngas Technologies Conference, Colorado Springs, CO, October 2017.
24. (**Invited**) Tadashi Ogitsu, "Computational design of novel catalyst system." Global Conference on Catalysis and Reaction Engineering 2017, Las Vegas, NV, October 19–21, 2017.
25. (**Invited**) Yanfa Yan, "New materials for photoelectrochemical water splitting," 232nd Electrochemical Society Meeting, National Harbor, MD, October 2, 2017.
26. Wei Wu, Dong Ding, and Ting He, "Development of high performance intermediate temperature proton-conducting solid oxide electrolysis cells," 232nd Electrochemical Society Meeting, National Harbor, MD, October 1–5, 2017.
27. (**Invited**) E.B. Stechel, "HydroGEN: Advanced Water Splitting Materials," International Workshop on Solar Thermochemistry, Julich, Germany, September 12–14, 2017.
28. Ting He and Dong Ding, "Perovskite Proton Conductors for Energy Conversion and Storage at Intermediate Temperatures," 20th Topical Meeting of the International Society of Electrochemistry, Buenos Aires, Argentina, March 19–22, 2017.

Collaborative Meetings Organized and Participated In

HydroGEN EMN Project Kick-Off Meeting

1. HydroGEN AWSM Project Kick-Off Meeting (>100 attendees), National Renewable Energy Laboratory, Golden, CO, November 14–15, 2018.

EMN-Wide Data Meeting

1. Application of Machine Learning and Data Analytics for Energy Materials Network Consortia 2018 (AMD4EMN 2018), organized by Y. Han, B. Wood, T. Ogitsu, HPCIC Innovation Center, Lawrence Livermore National Lab, Livermore, CA, May 2–3, 2018.

Benchmarking Meetings

1. HydroGEN AWSM Benchmarking Meeting (PEC Working Group Meeting), organized by CX Xiang, T. Deutsch, T. Ogitsu, and H. Dinh, Seattle, WA, May 13, 2018.
2. HydroGEN LTE/HTE Benchmarking Discussion, organized by K.E. Ayers, H. Dinh, and N. Danilovic, 233rd ECS Meeting, Seattle, WA, May 14, 2018.

Hydrogen Production Tech Team (HPTT) Review Meetings

1. HydroGEN Photoelectrochemical Water Splitting Project Reviews, Webinar, February 6, 2018.
2. HydroGEN Low Temperature Electrolysis Project Reviews, hosted by N. Danilovic and A. Weber, Lawrence Berkeley National Lab, Berkeley, CA, April 10, 2018.
3. HydroGEN Solar Thermochemical Water Splitting Project Reviews, Webinar, May 8, 2018.
4. HydroGEN High Temperature Electrolysis Project Reviews, planned to be at Idaho National Lab, Summer 2018.