HydroGEN Overview: A Consortium on Advanced Water Splitting Materials

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Presenter: Huyen Dinh, NREL

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Project ID # P148

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: $3.6M
• FY18 DOE funding: $9.9M
• FY19 planned DOE funding: $6.5M
• Total DOE funding received to date: $22M

Barriers

• Cost
• Efficiency
• Durability

Partners
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

https://energy.gov/eere/fuelcells/h2-scale
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 \( \text{H}_2 \) production, including:

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

**H\(_2\)** Production target <\$2/kg

HydroGEN consortium supports early stage R&D in \( \text{H}_2 \) 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/
Accomplishments: Updated Capability Nodes on the User-Friendly Node Search Engine for Stakeholders

Added **3 new** and updated **>40 current** capability nodes:
- Hybrid Organic Inorganic Perovskites for Water Splitting
- Understanding catalyst inks and ionomer dispersions
- Electronic-Structure Modeling for Atomistic Understanding of Catalytic Materials with Real-World Distributions of Facets and Defects

Considered capability assessment from benchmarking team

**Annual capability review is a rigorous process and keeps nodes updated and relevant**
Accomplishments: Maintained HydroGEN Website and Developed “Working with HydroGEN” Video Testimonials

Partner testimonial videos can be found here: https://www.youtube.com/watch?v=1eK8ZnVo2Y&list=PL3GM1pjrYAshur4Aoq1pojTC2cMPf8xs6P

Tom Jaramillo, principal investigator on a HydroGEN seedling project, talks about how the capabilities and expertise of the HydroGEN AWSM consortium can help researchers working on hydrogen technologies.
Accomplishments:
HydroGEN Data Hub: Making Digital Data Accessible

https://datahub.h2awsm.org/

179 Users
4055 Files

Cumulative Data on H2AWSM Data Hub

- Steadily adding more data,
- 44% of members participating

Data Hub implemented in May 2017
- Secure project space for team members
  - Centralized authentication
- Data publication process developed (FY2018Q3 QPM-see Reviewer-Only slides)
- Metadata tools and improvements to support advanced search

Types of Experimental Data

- 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 Publication Process

Create Dataset → Request to make Dataset Public → Steering Committee Review → Data Team Review → Set Public Flag → Verification

Data Team

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

HydroGEN: Advanced Water Splitting Materials
Accomplishments: Data Tools for Data Ingestion, Visualization and Analysis (Leveraging other EMNs)
5 currently available, 5 under development

Data Tools for
- EMN collaboration
  - Data exchange and exploration
  - Data analysis and visualization (A&V)
- External users
  - Access to comprehensive database
    - Experimental and computational
    - Materials properties
    - Spectroscopy, phase stability, etc.
  - Device performance

Organically linked data and their representations
Accomplishments: Technology Transfer Agreements (TT/A)

Streamlined Access

- **Four** standard, pre-approved TT/A between all consortium partners
- Executed all 21 project NDAs and 2 MTAs
- Updated multiple, more flexible CRADAs
  - Single Lab Single Participant
  - Multi-Lab Single Participant
  - Multi-Lab Multi-Participant
- Established Work For Others Agreements outside of FOA-awarded projects:
  - DeNora: GDE development on porous transport layers (LBNL Cell Testing Node)
  - German Aerospace Center: Concentrated solar power and solar fuels research (SNL)

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.
4 New NSF DMREF/DOE EERE HydroGEN EMN Projects
Collaboration/Accomplishments

NSF DMREF PSU LTE (IA023 Poster)

**PennState**

**Membrane Databases – New Schema and Dissemination**

**Recipient** Penn State University (PI: Michael A. Hickner)

**Subs** National Institute of Standards and Technology/NIST (PI: Debra Audus) and Rensselaer Polytechnic Institute/RPI (PI: Chulsung Bae)

**HydroGEN Node Experts**

National Renewable Energy Laboratory:

- Shaun Ali
- Guido Bender
- Kristin Munch
- Bryan Pivovar

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NSF DMREF PSU PEC (IA024 Poster)

**PennState**

**Experimental Validation of Designed Photocatalysts For Solar Water Splitting**

**Recipient** Penn State University (PI: Ismaila Dabo and Raymond E. Schaak)

**Subs** Cornell University (PI: Héctor D. Abrufia)

**HydroGEN Node Experts**

National Renewable Energy Laboratory:

- Todd Deutsch
- James Young

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NSF DMREF CSM STCH (IA022 Poster)

**High Temperature Defects: Linking Solar Thermochemical and Thermoelectric Materials**

**Recipient** Colorado School of Mines (PI: Eric Toberer and Vladan Stevanovic)

**Subs** University of Illinois Urbana-Champaign (PI: Elif Ertikin) and SLAC National Accelerator Laboratory (PI: Michael Toney)

**HydroGEN Node Experts**

National Renewable Energy Laboratory:

- Robert Bell
- David Girley
- Stephen Lany
- Philip Parilla

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NSF DMREF UB PEC (IA021 Poster)

**University at Buffalo**

**Collaborative Research: A Blueprint for Photocatalytic Water Splitting: Mapping Multidimensional Compositional Space to Simultaneously Optimize Thermodynamics and Kinetics**

**Recipient** University at Buffalo (PI: David Watsen)

**Subs** Texas A&M University (PI: Sarbajit Banerjee) and Binghamton University (PI: Louis Piper)

**HydroGEN Node Experts**

Lawrence Berkeley National Laboratory:

- Jinghua Guo
- David Prendergast

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Collaboration: HydroGEN FOA-Awarded Projects

16 projects passed GNGs and in phase 2 + 2 new HTE projects awarded

49 unique capabilities being utilized across six core labs

Advanced Electrolysis (10)
  LTE (5)
  HTE (5)

PEC (5)

STCH (5)
  2-Step MO_x (4)
  Hybrid Cycle (1)

Benchmarking & Protocols (1)
A Balanced AWSM R&D Portfolio
Accomplishments/Collaborations

Low Temperature Electrolysis (LTE)
(G. Bender: P148A; 5 Projects)

- PEM Electrolysis
  - PEM Component Integration
  - PGM-free OER and HER catalyst
  - Novel AEM and Ionomers
  - Electrodes

- AEM Electrolysis
  - PEM Electrolysis
  - AEM Electrolysis

High Temperature Electrolysis (HTE)
(R. Boardman: P148B; 5 Projects)

- O²⁻ conducting SOEC
  - Degradation mechanism at high current density operation
  - Nickelate-based electrode and scalable, all-ceramic stack design
  - High performing and durable electrocatalysts
  - Electrolyte and electrodes
  - Low cost electrolyte deposition
  - Metal supported cells

- H⁺ conducting SOEC

Photoelectrochemical (PEC)
(A. Weber: P148C; 5 Projects)

- 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: P148D; 5 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

HydroGEN: Advanced Water Splitting Materials

PEME = proton exchange membrane electrolysis;
AEME = alkaline exchange membrane electrolysis
PGM = platinum group metal
Solid oxide electrolysis cells: SOEC
Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

**Photoelectrochemical (PEC) Water Splitting**

UM achieved a *first demonstration of a functional Si/InGaN tandem photoelectrode*. A GaN/Si photocathode with stable operation (>100 h) at ~38 mA/cm², without using surface protection, was also demonstrated. UM is focused on developing Si-based, low cost, high efficiency (>15%), and stable (>1,000 h) PEC tandem water splitting devices, using scalable, low cost semi-conductors, nanowire tunnel junction, and N-rich GaN self-protection. The photoelectrodes were characterized and optimized by the NREL and LBNL nodes, while LLNL carried out modeling to understand the protection role of N-rich GaN surfaces.

**Low Temperature Electrolysis (LTE)**

NEU and UD demonstrated *high AEM electrolyzer performance* (0.46 A/cm² at 1.8 V, 85°C), using PGM-free Ni-Fe/Raney Ni OER and NiCr/C HER catalysts, PAP-TP-MQN AEM, and 1% K₂CO₃ solution, enabling durable, high-performing materials for efficient and low cost H₂ production. LBNL and SNL modeling nodes helped NEU better understand the AEM/catalyst interface, NREL nodes helped NEU characterize the membrane physical properties and optimize the catalyst formulation.
Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

High Temperature Electrolysis (HTE)
United Technologies Research Center (UTRC), with help from INL, LBNL, and NREL nodes, identified high performance proton-electrolytes and steam electrodes that resulted in 
button cell performance exceeding the DOE performance target, stable protective coatings for 500 h, and a cell model for SOEC performance characterization and cell/stack operation simulation. The HydroGEN nodes provided critical support by addressing technical barriers in metal alloy durability, electrode/electrolyte material optimization and stability, and SOEC modeling.

Solar Thermochemical (STCH) Water Splitting
CSM exceeded its hydrogen production target of 59 μmol H₂/g sample by producing 218 and 247 μmol H₂/g using two compositions within CeₓSr₂₋ₓMnO₄ family, x = 0.1 and 0.2, respectively. This promising performance further motivates the search for additional perovskite compounds with STCH water splitting properties. The objective is to discover new STCH materials that can meet steam to hydrogen efficiency of 20% and low cost H₂ production. The project leverages NREL and SNL modeling, material synthesis and characterization nodes.
Goal: 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.

Correlating Half- and Single- LTE Cells
Similar Ionomer Content Effect

- Ionomer content has a similar effect on MEA and half-cell performance
- Ionomer balance is needed for optimal performance

Ink Formulation and Electrode Processing
Affect SO₂ Electrolysis Performance

- Material exchange between NREL and SRNL
- Water-rich inks and slot-die-made MEAs performed better than alcohol-rich (R-OH) inks and gravure-prepared MEAs.

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

- Developed various model handoff requirements and interactions
  - Microkinetic model for OER pathways formulated
  - Initial barriers for OER on IrO$_2$ in acid calculated
- Experimental characterization of OER on IrO$_2$ (RDE, AP-XPS, ME) initiated
**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 cm$^2$ PEC panel.

**Accomplishments:** PV fabrication scale up from 0.1 to 1 cm$^2$
PEC vapor cell scale up from 1 to 4 cm$^2$
Benchmarking PEC cell performance between NREL and LBNL
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.

Accomplishments:
- First batch of YSZ-based SOEC fabricated using high-purity precursors.
- Sintering aid used in cathode buffer layers.
- Electrolyte thickness: 10-15 μm.
**STCH Supernode:** Develop Fundamental Understanding of the Mn-O Ligand Field’s Influence on Water Splitting (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.

**Accomplishments:**
- Develop synthetic routes to “ideal” Mn-O compounds
- Develop DFT methods to model core-hole spectroscopies
- Deploy operando test cell at SLAC (X-ray scattering)
- Conduct HR/STEM EELS studies on “ideal” compounds

**DFT** = Density functional theory  
**HR/STEM EELS** = high resolution/scanning transmission electron microscopy electron energy loss spectroscopy
Accomplishments: HydroGEN Benchmarking Advanced Water Splitting Technologies Project (P170)

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

Accomplishments:
• 1st Annual AWS community-wide benchmarking meeting (ASU, Oct. 24–25, 2018)
• 4 test frameworks developed
• 4 AWS technology surveys and result summaries published on the Data Hub
• 4 preliminary AWS roadmaps developed
• 1st round of test protocols defined and written
• Quarterly newsletters disseminated to AWS community
• >80 EMN capability nodes assessed; node gaps identified and communicated to HydroGEN

Goals:
• Develop standardized best practices for characterizing and benchmarking AWSMs
• Foundation for accelerated materials RD&D for broader AWS community
• Extensive collaboration and engagement with HydroGEN steering committee, node subject matter experts, and broad water splitting community

Development of Best Practices in Materials Characterization and Benchmarking: Critical to accelerate materials discovery and development
• The fact that about half of the 80+ nodes (capabilities) are being utilized suggests that the interaction with the HydroGEN-supported R&D projects/community is a benefit toward helping DOE realize its goals. It is unclear how to put into perspective the number of users, page views, downloads, etc., as well as the publications and presentations, and whether these are helping DOE achieve its goals/targets. As HydroGEN “matures,” a better metric would be clear evidence of how the nodes had an impact in making measurable/quantifiable benefits toward advancing R&D to meet DOE goals.

Response: We agree that testimonials and specific points of collaboration as witnessed by joint publications and presentations will be key in evaluating whether the nodes are providing critical or ancillary support for the FOA projects. Furthermore, cost reduction and technology maturity remain key metrics for success of the EMN.

• Probably one of the most pressing issues under Proposed Future Work is the development of an effective data management program, not so much in managing the data but in presenting to the R&D community in a format that is of value to the community. Developing benchmarking standard protocols and metrics is another pressing issue to make sure that the protocols for evaluating the various technologies provide an apples-to-apples comparison.

Response: We agree and are currently working on the data management in terms of dissemination with full metadata. In terms of protocols and metrics, this is an active area of work with the Benchmarking team lead by NEL/Proton OnSite, where HydroGEN core labs are actively engaged in helping to evaluate and establish the protocols.
Responses to Previous Year Reviewers’ Comments

• Some of the secondary, visible metrics, such as the use of the data hub (~250 data files in a year), should get more emphasis either on boosting participation or in communicating the complexity of the data contained within the hub. There is ambiguity as to what a single file contains: whether it is a single resistance measurement or a summary from an entire collection of measurements from a unique tool on the beamline. In short, if the scale of the databank were conveyed in person-hours per data file that makes up the ~250 total, that could strike an audience as more impressive/appropriate than leaving the number of files to remain as an abstract concept, which risks sounding underwhelming.

Response: There has been lots of activities in the data hub this past year, hence there are 2 slides on data, summarizing the publication process developed, the various tools that have been developed, and the type of data that are on the data hub (e.g., microscopy, pol curves, XRD, XPS). Each data file represents one of these data. We hope these two slides better communicate the level of participation and the complexity of the data in the Data Hub.

• Although individual projects have milestones and go/no-go points, the AWSM Consortium lacks clear success metrics at a higher level to guide its pathways and projects.

Response: The success metrics for the consortium are varied. The overall metric is cost reduction (through performance and durability gains) for the various water-splitting materials, remaining cognizant that they are at very different levels of technological maturity. Interactions and enabling the FOA projects is key to this and thus serves as metrics for the consortium. In addition, the existence of supernodes (with their more traditional research metrics, shown on FY19 Supernode Annual Milestones [AM] slide in “Reviewers Only slides”), the data analysis and data hub, and the research progress of individual nodes all provide further metrics for measuring success.
Proposed Future Work

• Core labs will execute HydroGEN nodes to enable successful phase 2 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
• Collaborate and perform integrated research in the 5 supernodes
• Integrate whole system (capability nodes, FOA awardees, data infrastructure, TT/A) 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, and other EMN, AE, PEC, and STCH communities
• Work closely with the Benchmarking Team to establish benchmarking, standard protocols, and metrics for the different water-splitting technologies
• 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

• 16 projects successfully passed GNG
• 5 new Supernodes
• 4 new NSF DMREF projects
• 2 new HTE projects
• 2 Work for Others agreements
• 5 new data tools; >4,000 files
• 4 partner testimonial videos
• 1 annual benchmarking workshop
• Multiple AWS standard protocols

HydroGEN fosters cross-cutting innovation using theory-guided applied materials R&D to advance all emerging water-splitting pathways for hydrogen production
Acknowledgements

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David Peterson  
James Vickers  
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| Maximilian Gorensek | Brenda Garcia-Diaz |
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HydroGEN
Advanced Water Splitting Materials

Energy Materials Network
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PEC Supernode Team

Best Practices in Materials Characterization

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Technical Backup Slides
Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

**Low Temperature Electrolysis (LTE)**
NREL’s contributed towards Proton Onsite achievement of 1.8 V at 2.0 A/cm², and 800 h PEM electrolysis durability at 2 A/cm², operating at 80°C and 30 bar. Proton’s improved cell efficiency is a step towards achieving its PEM water electrolysis cell efficiency goal of 43 kWh/kg (1.7 V at 90°C) and at a cost of $2/kg H₂, a significant improvement over the state-of-the-art cell efficiency of 53 kWh/kg.

**Photoelectrochemical (PEC) Water Splitting**
NREL’s high performance photoabsorber (GaInP₂/GaAs), integrated with Rutgers’ PGM-free electrocatalysts (LiCoO₂ and Ni₅P₄) and protection layer (TiN), achieved a solar-to-hydrogen efficiency of 11.5% for unassisted water splitting, on par performance with conventional PGM electrocatalysts (PtRu).

(NREL FY2018 Q4 AM – see Reviewer-Only slides)
Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

Low Temperature Electrolysis (LTE)
ANL demonstrated a 25% improvement in PEM electrolysis cell performance (310 mA/cm² at 1.8 V), using PGM-free Co-ZIF derived OER and Pt/C HER catalysts, N115 membrane, 60°C & 10 psi DI water, enabling the goal to reduce the anode catalyst cost by > 20 folds for the widespread implementation of PEME H₂ production. LBNL, LLNL, NREL, and SNL modeling, XPS, and microscopy nodes, respectively, contributed towards this achievement.

Photoelectrochemical (PEC) Water Splitting
SU demonstrated unassisted PEC water-splitting with PGM-free MoS₂ HER catalyst that achieved solar-to-hydrogen (STH) efficiency > 5% under 1 sun, providing a viable path for achieving low cost, stable and high (20%) STH PEC devices through earth-abundant protective catalysts, novel growth schemes, and new tandem III-V/Si system that has the potential to dramatically reduce H₂ production cost. The project leverages the NREL III-V fabrication, PEC characterization, corrosion, and on-sun testing expertise.
Accomplishments/Collaborations:
HydroGEN Collaborative R&D Technical Highlights

Low Temperature Electrolysis (LTE)
LANL demonstrated 4x higher in water-fed AEM electrolyzer performance (0.243 A/cm² at 1.8 V), compared to FY2018, using LANL developed carbon-free and PGM-free perovskite OER catalyst and SNL AEM membrane. The goal is to achieve low cost H₂ production via high performing, durable, and low cost PGM-free catalyst AEM electrolysis. NREL XPS and in-situ testing nodes helped LANL understand the OER catalyst surface composition and MEA electrode performance.

LANL and RPI prepared semi-crystalline AEM membranes, by acid catalyzed polymerization & without using expensive metal catalyst, that exceeded all of the project’s (and state-of-the-art) membrane conductivity, alkaline stability, and mechanical strength targets, as validated by LBNL characterization and modeling nodes. The goal is to synthesize and demonstrate high performing, durable, and economically-affordable AEMs in water-fed AEM electrolysis.

**Properties**
- IEC = 1.71 mequiv./g
- Water uptake = 144 %
- In-plane swelling = 30%

<table>
<thead>
<tr>
<th>Properties</th>
<th>Target</th>
<th>Status</th>
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<tbody>
<tr>
<td>Hydroxide conductivity (mS cm⁻¹) at 30 °C</td>
<td>40</td>
<td>42 (30 °C)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>54 (60 °C)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>63 (80 °C)</td>
</tr>
<tr>
<td>Alkaline stability after 300 h in 1 M NaOH at 80 °C</td>
<td>&lt; 5 % loss conductivity</td>
<td>0% loss</td>
</tr>
<tr>
<td>Mechanical toughness (MPa × % elongation) at 50 °C, 90% RH</td>
<td>&gt; 1400</td>
<td>2091</td>
</tr>
</tbody>
</table>
High Temperature Electrolysis (HTE)

Using Northwestern University catalyst, YSZ electrolyte \((\text{ZrO}_2)_{0.92}\text{(Y}_2\text{O}_3)_{0.08}\), and LBNL Metal-Supported Solid Oxide Cell and INL Advanced HTE testing nodes, the collaboration demonstrated a metal-supported SOEC for the first time in electrolysis mode, with the highest performance for oxygen-conducting type electrolysis cells to-date and promising stability.

Solar Thermochemical (STCH) Water Splitting

The University of Colorado Boulder, with NREL’s DFT node, developed and applied machine learning (ML) to accelerate STCH materials discovery, identifying several hundred stable STCH perovskites from over 1.1 million possible candidates, with 92% accuracy. SNL’s stagnation flow reactor and High-Temperature XRD nodes were used to experimentally validate water splitting kinetics and crystal structures for a select number of materials, providing critical feedback to develop rapid kinetic screening techniques of materials. Four materials have also been demonstrated to have \(\text{H}_2\) productions \(>200\ \mu\text{mol/g/cycle}\) at \(T_{\text{red}}=1450^\circ\text{C}\) and \(\Delta T=250^\circ\text{C}\), and results compared to computational predictions.
Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

**Photoelectrochemical (PEC) Water Splitting**

UH improved chalcopyrite stability in aqueous electrolyte by demonstrating **500 h of continuous operation at > 5 mA/cm²**, using a thin WO₃ coating on a high bandgap copper chalcopyrite, 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 STH efficiency > 10%. This project is supported by NREL synthesis and advanced characterization and LLNL modeling expertise to accelerate the development of materials and interfaces.

NSF-DMREF / DOE EERE HydroGEN EMN

Example:

Photoelectrochemical (PEC) Water Splitting
Reviewer-Only Slides
## FY19 NREL AOP Milestones

<table>
<thead>
<tr>
<th>Milestone Name/Description</th>
<th>End Date</th>
<th>Type</th>
<th>Status</th>
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</thead>
<tbody>
<tr>
<td>Kick-start the three NSF DMREF projects that NREL is supporting (PSU PEC, PSU LTE, and CSM STCH) and integrate them into HydroGEN.</td>
<td>12/31/2018</td>
<td>Q1 QPM</td>
<td>Complete</td>
</tr>
<tr>
<td>Initiate the 5 supernode efforts including a joint virtual kick-off meeting for each one. (NREL, LBNL, SNL, LLNL, INL, SRNL).</td>
<td>3/31/2019</td>
<td>Q2 QPM</td>
<td>Complete</td>
</tr>
<tr>
<td>Integrate new services into the Data Hub, including centralized authorization and sample management functions. Much of the HydroGEN research hinges on aligning and associating characterization and modeling data to uniquely identified samples. We will implement a sample management service into the Data Hub, which will include a backend database, an API layer and a data security layer. For centralized authorization, we will implement the Cognito Authentication service into the Data Hub, enabling 2-factor authentication consistently across all EMN data hubs.</td>
<td>6/30/2019</td>
<td>Q3 QPM</td>
<td>On Track (central authorization is complete)</td>
</tr>
<tr>
<td>Quantify the relationship between the exchange current density, specific activity and electrochemical surface area of a standard LTE OER catalyst via RDE with in-situ performance for at least 3 different electrode processing conditions and/or compositions, with properties comparable to IrO2 (mass exchange current density = 0.075 mA/mg, ECA = 28.7 m2/g and specific exchange current density = 0.26 µA/cm2). (LTE/Hybrid Supernode Milestone)</td>
<td>9/30/2019</td>
<td>Q4 Annual Milestone</td>
<td>On Track</td>
</tr>
<tr>
<td>Milestone Name/Description</td>
<td>Supernode/Lab AOP</td>
<td>Type</td>
<td>Status</td>
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<tr>
<td>Compare the exchange current density, specific activity and electrochemical surface area of a standard Hybrid Sulfur Cycle anode electro-catalyst via RDE with in-situ performance for at least 3 different electrode processing conditions and/or compositions with the goal of approaching 50-60% agreement between ex-situ and in-situ test.</td>
<td>LTE/Hybrid SRNL</td>
<td>Q4 AM 9/30/2019</td>
<td>On Track</td>
</tr>
<tr>
<td>Multiscale model predicts dominant reaction pathway with overall reaction rates in agreement within 10% error with experimental data for OER on IrO₂ under acidic conditions at two different applied overpotentials.</td>
<td>OER LBNL &amp; LLNL</td>
<td>Q4 AM 9/30/2019</td>
<td>On Track</td>
</tr>
<tr>
<td>The synthesized microstructures of 4-6 electrode/electrolyte pure phase material will be analyzed to confirm repeatability of microstructure and composition via microscopy and X-ray diffraction analysis. The materials will have no secondary phases and the microstructure will have porosity and pore size within 10% of each other.</td>
<td>HTE INL</td>
<td>Q4 AM 9/30/2019</td>
<td>On Track</td>
</tr>
<tr>
<td>Identify one or more Mn-O baseline systems sharing key characteristics with BCM, which produces 3x more hydrogen than CeO₂ when reduced at 1350°C and maintains higher water splitting favorability than SLMA at low oxygen partial pressure (&gt;50 umole/g at H₂O/H₂ ratio&lt;500). Data from SNL nodes will support first principles model development and refinement activities.</td>
<td>STCH SNL</td>
<td>Q4 AM 9/30/2019</td>
<td>On Track</td>
</tr>
<tr>
<td>Measure efficiency and durability a device of 8 cm² or larger area using a flexible-platform photoreactor equipped with multiple in-situ diagnostic techniques on 2-axis tractor for 2+ days.</td>
<td>PEC LBNL &amp; NREL (not in AOP)</td>
<td>Q4 AM 9/30/2019</td>
<td>On Track</td>
</tr>
</tbody>
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## FY18 AOP Milestones

<table>
<thead>
<tr>
<th>Milestone Name/Description</th>
<th>End Date</th>
<th>Type</th>
<th>Status</th>
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</thead>
<tbody>
<tr>
<td>Organize and host a HydroGEN project kick-off meeting for the 19 new FOA awardees and the 6 core lab members to help integrate them into the EMN.</td>
<td>12/31/2017</td>
<td>QPM</td>
<td>Complete Nov. 2017</td>
</tr>
<tr>
<td>80 HydroGEN capabilities reviewed based on developed process and evaluation criteria (e.g., utilization across the 18 new FOA projects).</td>
<td>3/30/2018</td>
<td>Annual Milestone</td>
<td>Complete</td>
</tr>
<tr>
<td>Integrate a data publication process into the data hub, enabling methods for assigning DOIs to uniquely identify public datasets and processes for approving and sharing data with the public.</td>
<td>6/30/2018</td>
<td>QPM</td>
<td>Complete (slide 10)</td>
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<tr>
<td>Benchmark solar-to-hydrogen efficiency of best-in-class LiCoO2 anode and Ni5P4 cathode catalysts integrated on an upright GaInP2/GaAs tandem cell with a target of greater than 10%.</td>
<td>9/30/2018</td>
<td>QPM</td>
<td>Complete (slide 39)</td>
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Publications


Presentations


Presentations

20. G.C. Dismukes, “Bioinspired heterogeneous electrocatalysts for CO2 reduction and water splitting: Energy-efficient C-C coupling rivaling enzymes,” Leiden University, Institute of Chemistry, Leiden, the Netherlands, Danish Technical University, Institute of Physics, Copenhagen, DK, Aarhus University, iNano, Aarhus, DK, October 2018.


Presentations

27. D. Ding. “Development of Electrochemical Processing and Electrocatalysis at Intermediate Temperatures at Idaho National Laboratory (INL),” Invited Lecture for faculty and graduate students, Department of Mechanical and Aerospace, West Virginia University, Morgantown, WV, USA, Dec. 4, 2018.


30. D. Ding, “Advancement of Intermediate Temperature Solid Oxide Energy Conversion Technologies at Idaho National Laboratory.” Invited Lecture for faculty and graduate students, Department of Chemical Engineering, University of Louisiana at Lafayette, Lafayette, LA, USA, April 1, 2019.


Presentations


Presentations


Presentations


Presentations


Presentations


