Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

HydroGEN Overview:
A Consortium on Advanced Water Splitting Materials

PIs: Huyen Dinh, Shaun Alia, Bryan Pivovar (NREL); Joel Ager, Adam Weber (LBNL); Dong Ding, Qian (Jennifer) Zhang (INL); Anthony McDaniel, Sean Bishop (SNL); Tadashi Ogitsu, Brandon Wood (LLNL)

Presenter: Huyen Dinh, National Renewable Energy Laboratory (NREL)

DOE project (AOP WBS#): 2.7.0.518 (HydroGEN 2.0) & 2.7.0.513 (Node Support)

Date: May 7, 2024

DOE Hydrogen Program

2024 Annual Merit Review and Peer Evaluation Meeting

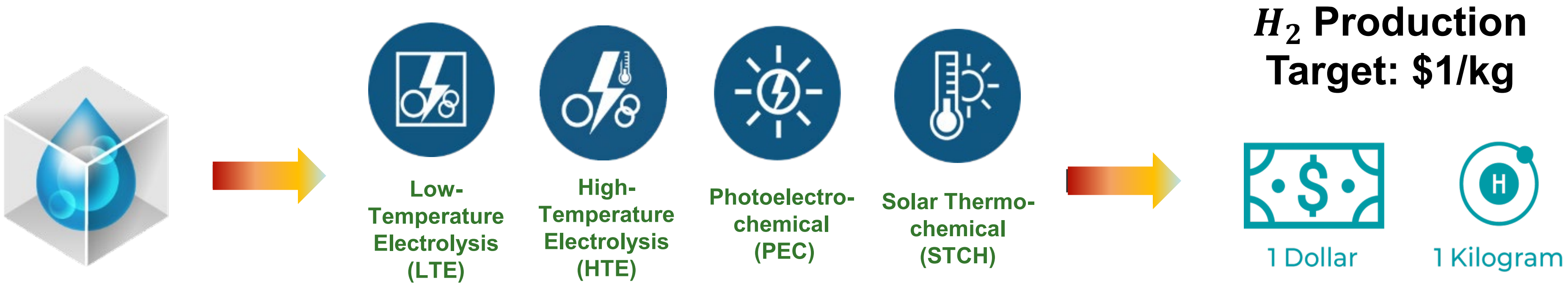
Project ID # P148

NREL Transforming ENERGY | BERKELEY LAB Bringing Science Solutions to the World | Sandia National Laboratories | INL Idaho National Laboratory | Lawrence Livermore National Laboratory

Project Goal

Website: https://www.h2awsm.org/

Goal: Accelerate foundational R&D of innovative materials for advanced water splitting (AWS) technologies to enable clean, sustainable, and low-cost ($1/kg H_2) hydrogen production.



HydroGEN is focused on early-stage R&D in H_2 production and fosters cross-cutting innovation using theory-guided applied materials R&D to advance all emerging water-splitting pathways for hydrogen production

HydroGEN Overview

Timeline and Budget

Total DOE funding since June 2016 launch: $61.8M

- **FY16** — DOE Funding: $2M
- **FY17** — DOE Funding: $3.5M
- **FY18** — DOE Funding: $9.9M
- **FY19** — DOE Funding: $8.4M
- **FY20** — DOE Funding: $13.175M
- **FY21** — DOE Funding: $5.7M
- **FY22** — DOE Funding: $9.6M
- **FY23** — DOE Funding: $10.2M
- **FY24** — **DOE Funding: $9.6M**
  Core Lab R&D ($5.1M)
  FOA & Lab-Awarded Prjt. Support ($4.5M)

Barriers

- **Cost**
- **Efficiency**
- **Durability**

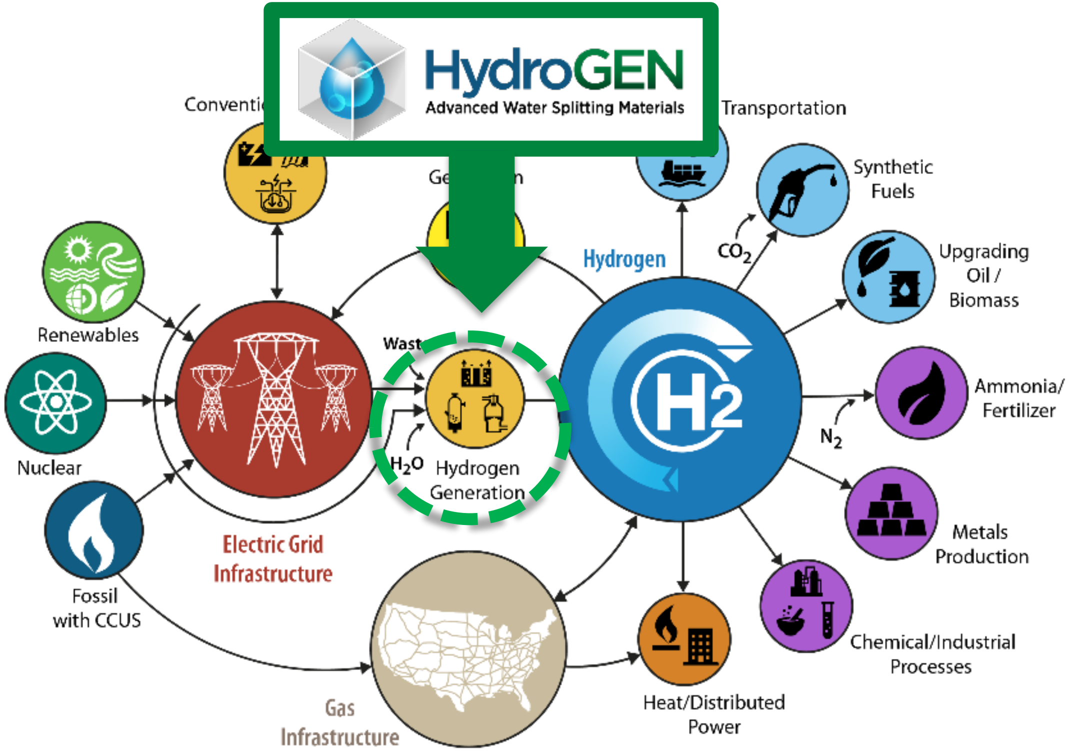
Partners

National Lab Consortium Team*

NREL Transforming ENERGY
Lawrence Livermore National Laboratory
Sandia National Laboratories
INL Idaho National Laboratory
BERKELEY LAB

* Expansion adds additional university and industrial partners through FOA (2922, Topic 3) projects and Lab Call

HydroGEN connection to H2@Scale: Enabling Affordable, Reliable, Clean and Secure Energy
Relevance and Impact



Transportation and Beyond

- Large-scale, low-cost hydrogen from diverse domestic resources enables an economically competitive and environmentally beneficial future energy system across sectors
- Hydrogen can address specific applications that are hard to decarbonize
- Today: 10 MMT H2 in the US
- Economic potential: 2x to 4x more

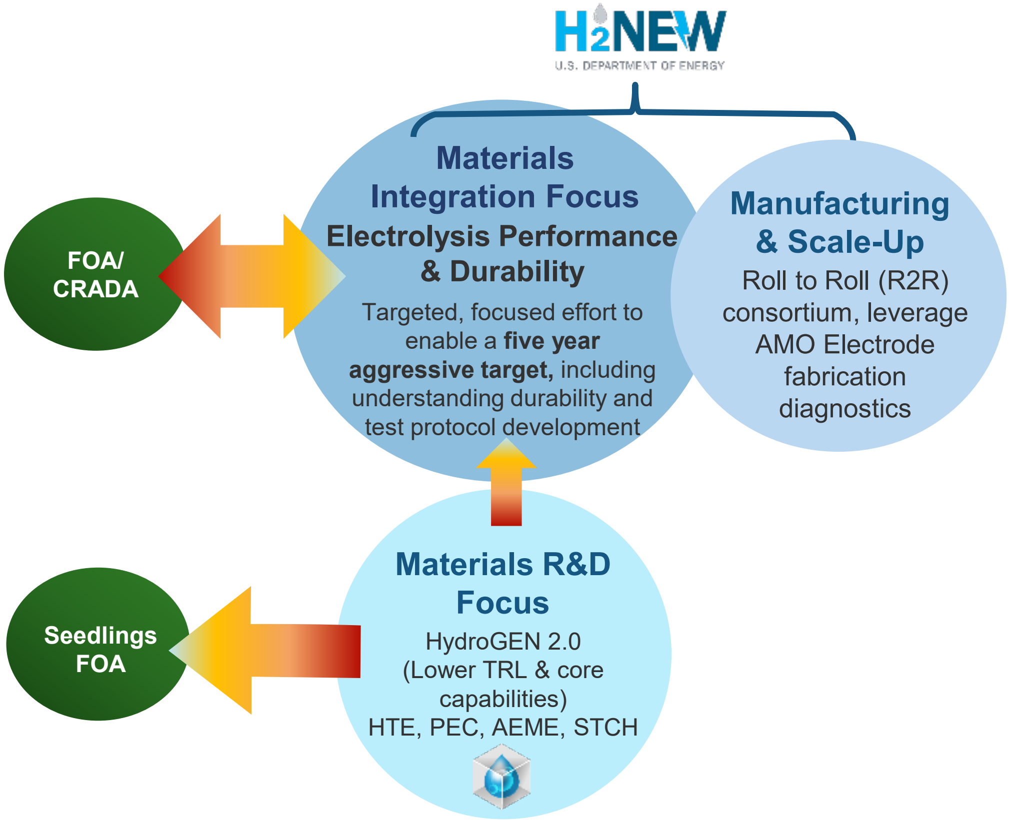
Materials innovations are key to enhancing performance, durability, and reduce cost of hydrogen generation, storage, distribution, and utilization technologies key to H2@Scale

"Hydrogen at Scale (H_2@Scale): Key to a Clean, Economic, and Sustainable Energy System," Bryan Pivovar, Neha Rustagi, Sunita Satyapal, *Electrochem. Soc. Interface* Spring 2018 27(1): 47-52; doi:10.1149/2.F04181if.

Source: DOE Hydrogen and Fuel Cell Technologies Office, https://energy.gov/eere/fuelcells/h2-scale

HydroGEN Materials R&D Feeds to H2NEW Materials Integration

Approach and Relevance



H2NEW

- Polymer electrolyte membrane (PEM) water electrolysis
- Oxygen-conducting solid oxide water electrolysis (SOEC)

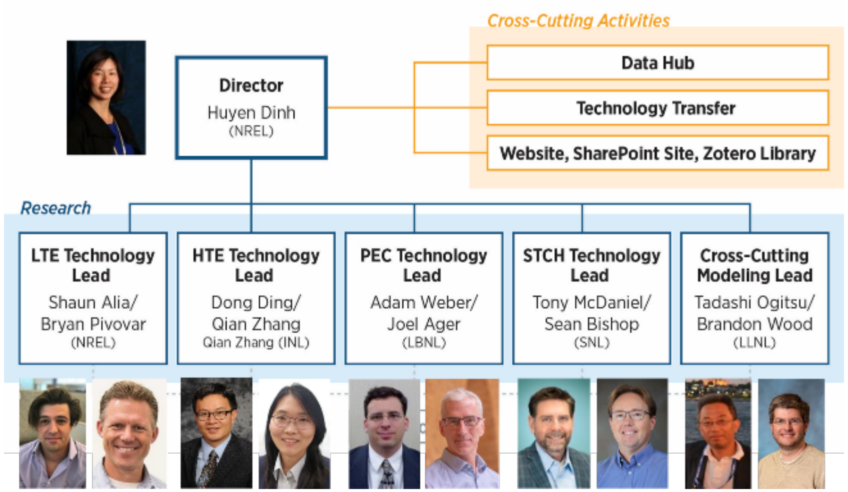
HydroGEN 2.0 (lower TRL AWS)

- Alkaline exchange membrane (AEM) water electrolysis
- Metal-supported SOEC (MS-SOEC)
- Proton-conducting SOEC (p-SOEC)
- Photoelectrochemical (PEC)
- Solar thermochemical (STCH)

HydroGEN Lab R&D + Lab Capability Support

EMN Collaboration and Approaches

Lab R&D
Early-Stage Materials R&D Projects



NREL Transforming ENERGY | INL Idaho National Laboratory | BERKELEY LAB | Sandia National Laboratories | Lawrence Livermore National Laboratory

+

Lab Support
Lab capabilities + experts support early-stage materials R&D projects

HydroGEN Materials Capability Network
55 Lab- and FOA-awarded Projects

LTE Node Labs
NREL National Renewable Energy Laboratory
BERKELEY LAB
Sandia National Laboratories
Lawrence Livermore National Laboratory

Support through:
Personnel
Equipment
Expertise
Capability
Materials
Data

LTE FOA Projects
BERKELEY LAB
nel
Lawrence Livermore National Laboratory
ecolectro
Georgia Tech
Research Corporation

Please attend 5 the HydroGEN technology-specific AMR posters (p148a, b, c, d, e) (https://www.hydrogen.energy.gov/amr-presentation-database.html) for more details.

Lab Capability Support of 24 New "Seedling" Projects

EMN Collaboration and Approaches

5 AEME projects: 3 FOA-awarded projects & 2 Lab-call awarded projects

LTE Node Labs
- NREL National Renewable Energy Laboratory
- Berkeley Lab
- Sandia National Laboratories
- Lawrence Livermore National Laboratory

Support through: Personnel, Equipment, Expertise, Capability, Materials, Data

LTE FOA Projects
- Berkeley Lab
- nel
- Lawrence Livermore National Laboratory
- ecolectro
- Georgia Tech Research Corporation

6 p-SOEC projects : 4 FOA-awarded projects & 2 Lab-call awarded projects

HTE Node Labs
- INL Idaho National Laboratory
- NREL Transforming ENERGY
- Sandia National Laboratories
- Berkeley Lab
- Lawrence Livermore National Laboratory

Support through: Personnel, Equipment, Expertise, Capability, Materials, Data

Interactive HTE Projects
- Raytheon Technologies
- West Virginia University
- Georgia Institute of Technology
- Colorado School of Mines
- The University of Oklahoma
- Lawrence Livermore National Laboratory

6 PEC FOA-awarded projects

PEC Node Labs
- NREL National Renewable Energy Laboratory
- Berkeley Lab
- Lawrence Livermore National Laboratory

Support through: Personnel, Equipment, Expertise/Protocols, Capability, Materials/cells, Data

Interactive PEC projects
- Rice
- Yale
- California Institute of Technology
- The University of Toledo
- University of Michigan
- University of Hawai'i

5 STCH FOA-awarded projects

STCH Node Labs
- Sandia National Laboratories
- INL Idaho National Laboratory
- Lawrence Livermore National Laboratory
- NREL National Renewable Energy Laboratory

Support through: Personnel, Equipment, Expertise, Capability, Materials, Data

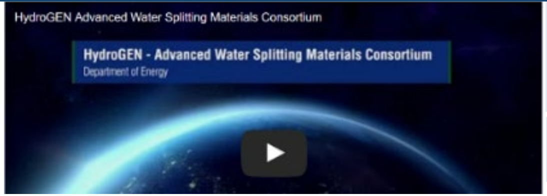
Interactive STCH Projects
- Arizona State University
- University of Colorado Boulder
- Massachusetts Institute of Technology
- Washington University in St. Louis
- Saint-Gobain

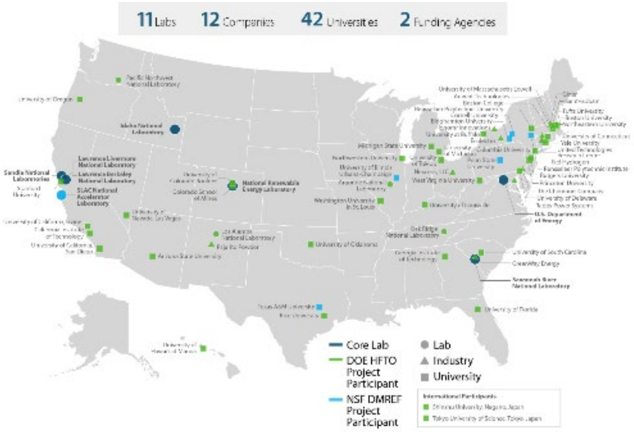
6 PEC and 5 STCH FOA-awarded projects have AMR presentations (https://www.hydrogen.energy.gov/amr-presentation-database.html). Some project technical accomplishments are highlighted in this presentation.

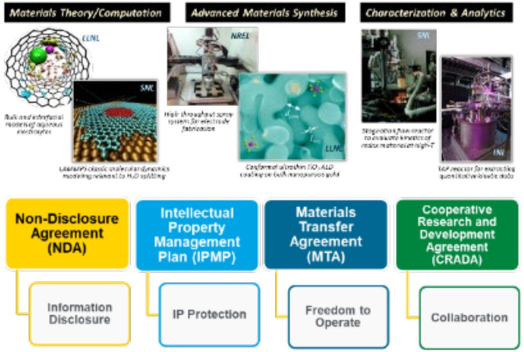
Effectiveness of HydroGEN EMN Framework

Collaboration / Accomplishments, Streamline Access

HydroGEN is vastly collaborative, has produced many high value products, and is disseminating them to the R&D community.







https://www.h2awsm.org/working-with-hydrogen

- 245 Publications, Impact factor* = 2.66
  8,771 citations, 669 authors
- 5 community benchmarking workshops
- 44 project NDAs, 2 MTAs
- 46 capabilities utilized across 6 labs
- STEM Work Force Development
- Diverse leadership and community
- Kick-off Meeting for 11 new projects
- Joined IEA Hydrogen TCP – Task 45
  Renewable hydrogen Subtask 2 PEC

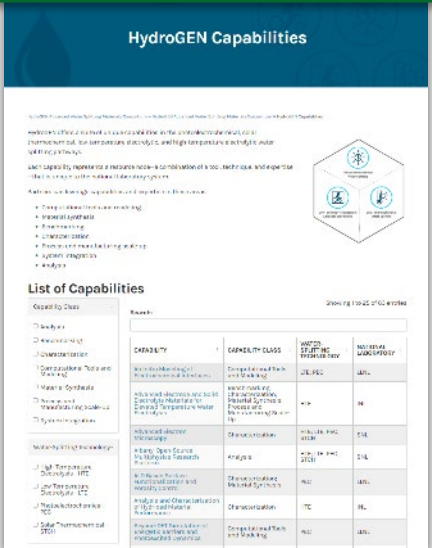
*Field-weighted citation impact (FWCI) indicates how the number of citations received by the Publication Set's publications compares with the average number of citations received by all other similar publications in Scopus.

Effectiveness of HydroGEN EMN Framework: Website Outreach

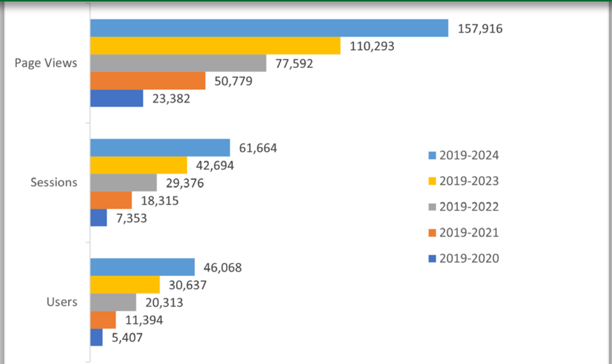
New website launched March 2024:
www.energy.gov/eere/h2awsm

Upgraded website platform and hosting environment

Website connects users to capabilities, publications, Data Hub, news, and more with greater security, new dynamic features, and more efficient content management



Cumulative website usage shows continued engagement



News articles highlight research and accomplishments

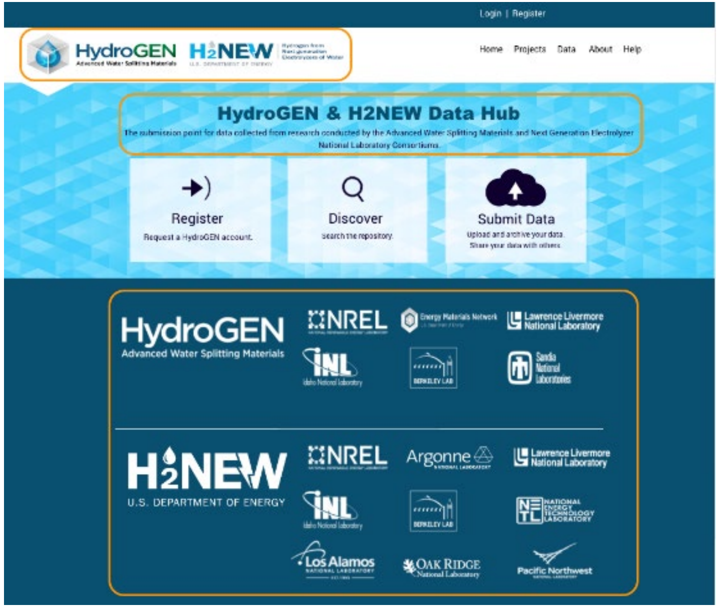
Collaborative HydroGEN and H2NEW Data Hub

Collaboration / Accomplishments

Making Digital Data Accessible

1. **Data repository**
   - Storage and sharing of research data: public vs. private data
2. **DOI/Publication of data**
   - Internal vs. external data
3. **Provide security mechanisms**
   - User login
   - Project level access management
4. **Maintain security compliance**
5. **Visualization and analysis capabilities**

Incorporated H2NEW branding and projects into the Data Hub



Front End

- Addition of H2NEW primary and contributor logos
- Primary tagline description change to include H2NEW

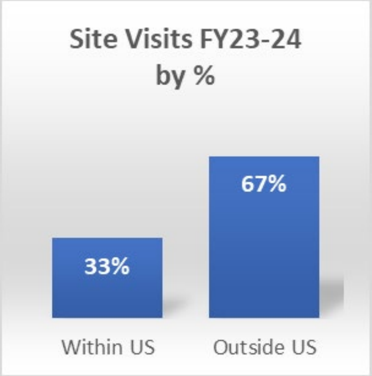
Data

- H2NEW Project Creation

Effectiveness of HydroGEN EMN Framework:
Collaboration / Accomplishments

https://datahub.h2awsm.org/

Growing & active user community



	Site Visitors	New Visitors	Returning Visitors
FYTD 2024	4,786	4,715	71

FY23-FYTD	New Projects
H2NEW	9
New FOA projects	11
Other new projects	7

H2NEW & HydroGEN Engagement

Data Hub Team 2023-2024 to date in Review
- 2024 Cyber Security Upgrade release complete.
- Incorporated H2NEW into the HydroGEN Data Hub, including branding and projects.
- Progress in development work for future search capabilities.
- Continues to support the authorization and management of user accounts, the user interface, project creation and structure, and dataset upload and publication

	Users	Projects	Datasets	Files
Project thru FY23	469	87	483	6,191
Project thru FY24 (FYTD)	503	88	500	6,261
% change in FY24	38%	44%	9%	51%

Many Types of Experimental Data

Material characterization
- XRD, SFR, XPS, XRF, SEM, TEM, Raman , SIMS, Solar Furnace Reactor

Device performance
- Electrolysis, PEC J-V, IPCE, Tafel plots

Materials durability data
- TGA, membrane conductivity

Community Approach to Benchmarking and Protocol Development for AWS Technologies
Collaboration / Accomplishments

Pacific Northwest NATIONAL LABORATORY · nel · ASU Arizona State University · Caltech

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

Best Practices in Materials Characterization

Kathy Ayers, Nel Hydrogen (LTE)
Ellen B. Stechel, ASU (STCH)
Olga Marina, PNNL (HTE)
CX Xiang, Caltech (PEC)
Consultant: Karl Gross, George Roberts

- Strong community engagement and participation, nationally and internationally
  - Participation from both HydroGEN and H2NEW consortia
- Disseminated information to AWS community via HydroGEN Data Hub, website, SharePoint site, email, quarterly newsletters, workshops

Accomplishments

- 20 standardized measurement protocols and benchmarks published in open-access journal Frontiers in Energy Research special issue: free to download: https://www.frontiersin.org/research-topics/16823/advanced-water-splitting-technologies-development-best-practices-and-protocols#articles
  - 8 LTE, 4 HTE, 5 PEC, 3 STCH
  - 11k total downloads and 70k views
- Published 15 LTE protocols on the Data Hub
- 5 Annual AWS community-wide benchmarking workshop
- Developed high-level roadmaps by AWS technology
- Initiated validation of 2 LTE protocols (LANL, NREL, UO)

Validation of AEMWE Testing Protocols

Accomplishments & Progress

P170

Validation Goals: Ensure each protocol can be universally applied across the AWST community to produce repeatable results that can be reported and compared;

Current LTE validation sites: LANL, NREL, University of Oregon, coordinated by NEL

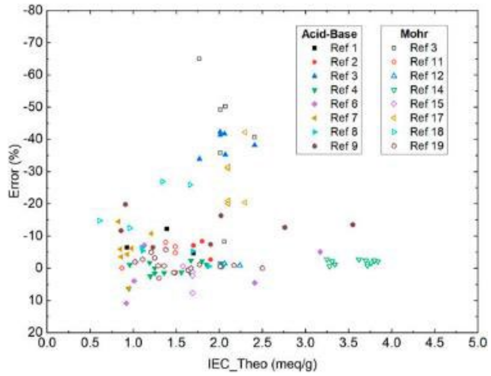
Test Protocols Validation in Process:

1. Ion Exchange Capacity (IEC)
   - LTE-P-7 SOP on the HydroGEN Data Hub
   - Standard Operating Protocols for Ion-Exchange Capacity of Anion Exchange Membranes, Frontiers in Energy Research Journal, Vol 10 – 2022. (7,539 views, 1,050 downloads) https://doi.org/10.3389/fenrg.2022.887893
2. Alkaline Stability of AEMs
   - LTE-P-22 SOP on the HydroGEN Data Hub
   - Assessing the Oxidative Stability of Anion Exchange Membranes in Oxygen Saturated Aqueous Alkaline Solutions, Frontiers in Energy Research Journal, Vol 10 – 2022.(3,215 views, 675 downloads) https://doi.org/10.3389/fenrg.2022.871851

Validation site example: Leverage HydroGEN Consortium Capabilities

HydroGEN Advanced Water Splitting Materials

NREL, LBNL, SNL, INL, and LLNL



Summary of Errors versus Theoretical IEC values from typical aggregated from the AEMs reported. (https://doi.org/10.3389/fenrg.2022.887893)

Safety Planning and Culture
Approach

- HydroGEN is **NOT** required to submit a safety plan for review by the Hydrogen Safety Panel
- Every National Lab has a rigorous DOE-approved Safety Procedure which is regularly reviewed and monitored by cognizant DOE Field Offices
  - **NREL:** Work Planning and Control (WPC) which uses Integrated Safety Management (ISM)
  - **LBNL:** WPC with ISM
  - **INL:** Integrated Safety Management System (ISMS)
  - **SNL:** WPC with ISM
  - **LLNL:** ISMS

Integrated Safety Management (ISM) Process can be described:

- Define the scope of work
- Analyze hazards associated with the work
- Develop and implement hazard controls
- Perform work within controls
- Provide feedback and continuous improvement

Engineered Control Strategies Utilized *For Hydrogen*

- ***Prevent a release***—Use high quality stainless steel tubing, fittings, and components to resist hydrogen embrittlement;
- ***Detection***—use robust point and area detection to detect leaks***;***
- ***Process control***—interlock detection system with process controls to shut off system; low-V heat tape controllers
- ***Ventilation***—robust ventilation to quickly evacuate areas***;***
- ***Control of ignition sources***—use protected electrical systems that prevent gas ignitions; over-temperature protection for heat tapes
- ***Defense in depth.*** Uses layers of controls in the design. For instance, the ventilation system design for hydrogen generation laboratory is redundant so if one exhaust system fails a redundant system will take the load.

Safety Culture Principles

- Everyone is personally responsible for ensuring safe operations
- Leaders value the safety legacy they create
- Staff raise safety concerns because trust permeates the organization
- A questioning attitude is cultivated
- Learning does not stop.
- Hazards are identified and evaluated for every task, every time
- A healthy respect is maintained for what can go wrong

DEIA/Community Benefits Plans and Activities

- HydroGEN is NOT required currently to have DEIA/Community Benefits Plans
  - Recruited Graduate Education Minority (GEM), Student Trained in Applied Research (STAR), and Science Undergraduate Laboratory Internship (SULI) summer interns to work at NREL
  - NREL and University of Puerto Rico, Mayaguez kicked off a seminar series called Un Cafecito Puerto Rico con Puerto Rico to spur collaboration between the island and NREL.
  - Mentored graduate students, postdocs, and early career researchers to chair conference sessions (244th ECS Meeting, I06 Symposium)
  - Invited diverse researchers (e.g., early career, female) to give talks at conference
  - Posted open positions to attract diverse applicant pool (NSBE, AWS, AABE, NAAAP, etc.)
  - Plan to develop DEIA/Community Benefits Plans. Some activities may include:
    - Plan to participate in Faculty Applied Clean Energy Science (FACES) - Visiting Faculty Program with a professor at a minority serving institution (MSI)
    - Plan to incorporate DEIA minute at HydroGEN meetings
    - Plan to visit MSIs to give talks about hydrogen and recruit students

- 11 new FOA-awarded HydroGEN projects have DEIA/Community Benefits Plans
  - Hold research seminars and/or outreach events to educate undergraduates from MSIs
  - Recruit &/or engage interns and staff from underrepresented groups (e.g., female, Navy veteran) and/or MSIs
  - Host onsite lab tours for K-12 students and instruct them on general AWS technologies
  - Achieve goal of > 50% participation (including senior personnel) by traditionally underrepresented groups (women, LGBTQ+)
  - Develop a program to engage Hispanic female students at the Community College level


Prithviraj Chumble (RPP) & Micah Mitchell (STAR)


John Carbo (SULI)


Melissa Kreider (Postdoc)


Cesar Lasalde-Ramirez (GEM)


Ai-Lin Chan (Researcher)


Sarah Blair (Postdoc)


Julia Lenef (Postdoc)


Noor Ul Hassan (Postdoc)


Samuel Koomson (Postdoc)

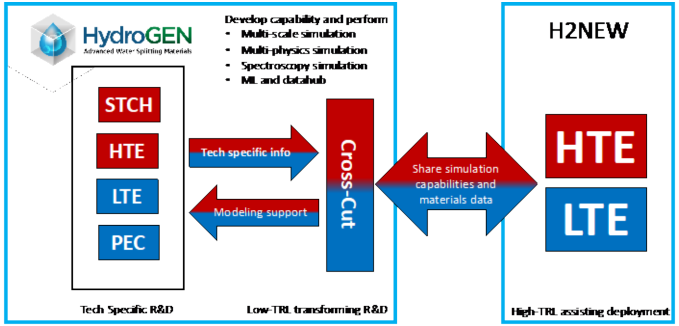

Joshua Gomez (Researcher)


Kiseok Oh (Postdoc)

Science Challenges for Impactful HydroGEN Lab R&D:
Approach

- ***LTE***: improve AEM electrolysis performance and durability by determining the role of supporting electrolyte and the limiting factors behind DI water operation
- ***HTE***:
  - **MS-SOEC**: improve performance and durability with a scaled-up cell
  - **p-SOEC**: understand the proton conduction and electronic leakage mechanisms of electrolyte materials in proton-conducting SOEC
- ***PEC***: materials stability and device durability
- ***STCH***: identify and understand how structural features, composition, and defect dynamics engender high capacity–high yield behavior in materials

Cross-Cutting Modeling: theory-guided design to analyze performance and durability of materials under simulated operating conditions



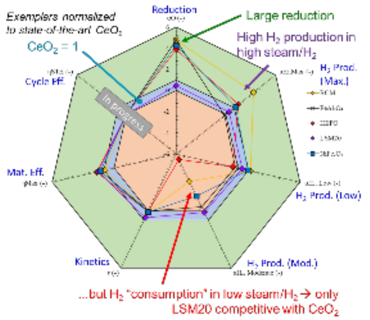
Responses to Previous Year Reviewers' Comments

In the future, the consortium can provide a year-to-year progress (since 2016) that would provide an overall outlook of the accomplishments.

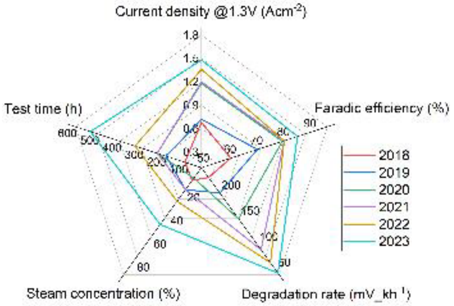
There are no clear roadmaps and targets for each technology.

- Metrics for each AWS technologies have been proposed to which new materials, devices, and/or systems can be benchmarked against and/or to track year-to-year progress. Performance, durability, and cost are integrated in the metrics.

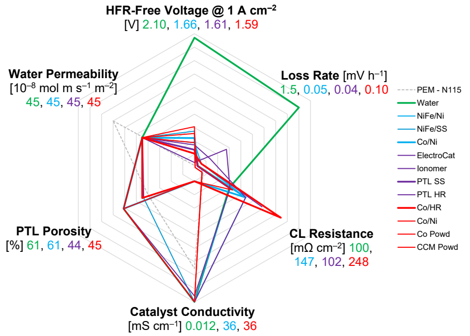
STCH



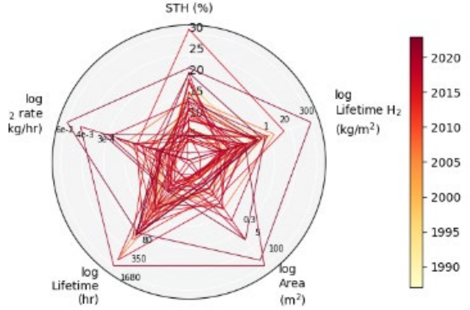
p-SOEC



AEMWE



PEC



Responses to Previous Year Reviewers' Comments

A focused research on degradation mechanisms is suggested. Degradation mechanisms studies should be planned. Most durability data was short, which limits the significance of project progress.

- We agree that improvements in durability are the key to advancing the technology readiness level. We intend to continue the focus on durability and sharing best practices and methods.
- Increased efforts in durability studies have been planned and are reflected in Accomplishments slides and the Q4 Milestone.
  - **AEMWE Lab R&D Q4 Milestone**: Testing of at least 3 membrane electrode assemblies with commercial materials for at least **500 h** to set a benchmark performance decay rate and understand relevant degradation processes. These tests will vary the materials evaluated and/or operation parameters, and leverage HydroGEN nodes to determine how losses are observed and the component/process involved.
  - **P-SOEC Lab R&D Q4 Milestone**: Develop effective approaches to suppress electronic leakage of electrolyte materials in p-SOEC. Criteria: Complete accumulative **>2000 hrs** test for p-SOEC and demonstrate a Faradaic efficiency degradation rate <1%/kh.
  - **PEC Lab R&D Q4 Milestone**: Stand-alone solar water splitting device of at least 4 cm^2 illuminated area capable of indoor and outdoor operation with neutral (pH ~ 7) water. Device is expected to generate visible bubbles of H_2. (NREL and LBNL). Criteria: Continuous operation of stand-alone solar water-splitting device for **100 hours** with remote monitoring by time-lapse photography. If hydrogen and oxygen generation rate is still 60% of initial performance, the testing will be extended to 500 hours.
  - Per the DOE requirement for **FOA-awarded seedlings projects**, long-term (multi-week) testing of materials **on-sun** is planned for **STCH (1 g H_2 / hour) and PEC (0.1 g/h for 2 weeks of diurnal operation).**

Responses to Previous Year Reviewers' Comments

It would be good to understand how technoeconomic analysis (TEA) is informing the choice of performance metrics so that there is a clearer focus on the critical ones.

- DOE HFTO has performed TEA of these early-stage AWS technologies in the past. This and the HydroGEN technology expertise provide the basis for identifying the materials R&D challenges, informing the R&D direction and developing the performance metrics proposed in FY2023. Updated TEA will be performed in the future.
- All five STCH seedling projects have requested TEA support from the NREL nodes: Techno-Economic Analysis of Hydrogen Production and Multi-scale modeling and STCH TEA. TEA support examples include:
    - Establish modeling tools to simulate reactor and system performance to guide design of future reactor iterations and identify cost implications associated with decoupling the reactor from the solar receiver via gas heating and thermal storage.
    - Develop a TEA framework of the perovskite-based STCH production using Reactor Train System developed by the project to size component and solar field layout for commercial scale integration including renewable sources and thermal energy storage and develop STCH system capital costs compatible with project system performance model and incorporate capital costs in H2A analysis tools.

Responses to Previous Year Reviewers' Comments

- *For the Data Hub, it is recommended that the project improve the ability to track data download and (if possible) information about who is downloading the data (industry versus academic, U.S. versus international, etc.) to better assess the success of this information-sharing vehicle.*
  - Events on the Data Hub that can currently be captured with google analytics:
    - *File downloads*: total events, unique events, individual file names, file type
    - *Outbound link clicks:* total events, unique events, address linked, dataset link was clicked from
  - We will work on improving the ability to track data download
- *It was not clear how the data quality was being evaluated, prior to being uploaded to the Data Hub.*
  - Data quality is not evaluated prior to be uploaded to the data hub. However, data quality is reviewed against specific standards and revised for quality by the data hub administrators, the HydroGEN steering committee prior to being made public. If data does not meet quality standards, it is not made public. Specific standards were developed by the data hub administrators and the Director of the HydroGEN EMN.

- **AWS Technology-specific reviewers' comments can be found in the HydroGEN AWS technology specific posters: p148a (LTE), p148b (HTE), p148c (PEC), p148d (STCH), p148d (crosscut modeling)**

Low Temperature Electrolysis (LTE) Technical Accomplishments: Shaun Alia

Participating Labs: NREL, LBNL, SNL

Project ID # P148A

LTE Lab R&D Team		
NREL Transforming ENERGY	BERKELEY LAB Bringing Science Solutions to the World	Sandia National Laboratories
Shaun Alia	Sarah Berlinger	Josh Sugar
Ai-Lin Chan	Tugrul Ertugrul	Jamie Trindell
Huyen Dinh	Jingjing Liu	Arielle Clauser
Mai-Anh Ha	Xiong Peng	
Melissa Kreider	Adam Weber	
Ross Larsen	Rito Yanagi	
Douglas Marsh		
Meital Shviro		
Emily Volk		

HydroGEN LTE Seedling Projects with Lab Capability Support

LTE Lab R&D Approach & Collaboration

HydroGEN LTE Projects

- Historically supported 8 FOA projects with 41 nodes
- LTE lab R&D involves 6 capability nodes
- Planning to support HydroGEN FOA-awarded (aka Seedlings) and Lab call projects

Support of Lab Call/FOA Projects

LTE Node Labs

NREL
NATIONAL RENEWABLE ENERGY LABORATORY
BERKELEY LAB
Sandia National Laboratories
Lawrence Livermore National Laboratory

Support through:

Personnel
Equipment
Expertise
Capability
Materials
Data

LTE FOA Projects

BERKELEY LAB
nel
Lawrence Livermore National Laboratory
ecolectro
Georgia Tech Research Corporation

New Lab-Call Awarded Projects:

1. ELY-BIL004: Hierarchical Electrode Design for Highly Efficient and Stable Anion Exchange Membrane Water Electrolyzers: LBNL
2. ELY-BIL005: Studying-Polymers-On a-Chip (SPOC): Increased Alkaline Stability in Anion Exchange Membranes: LLNL

New FOA-Awarded Projects:

1. Alkaline Stable Organic Cations Incorporated into Rigid Polymer Backbones for Enhanced Mechanical Properties of Thin Films: Ecolectro Inc.
2. Low-Cost, Clean AEM Electrolysis through Transport Property Understanding, Manufacturing Scale-up, and Optimization of Electrodes and Their Interfaces: Nel Hydrogen
3. Durable, Low-Cost, Manufacturable AEM Electrolyzer Components: Georgia Tech Research Corporation

Enabling High Efficiency, Durable AEM Electrolysis Performance

LTE Lab R&D Goals and Approach

NREL | BERKELEY LAB | Sandia National Laboratories | **6** Nodes

Goals: Determine the role of the supporting electrolyte and the limiting factors behind water operation in AEM electrolysis

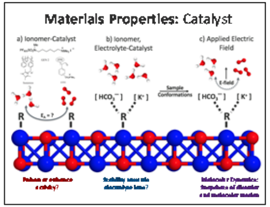
- Evaluate AEM's ability to approach PEM performance/durability
- Elucidate interactions at the ionomer/catalyst interface to assess ionomer stability and catalyst poisoning
- Understand the impact of catalyst layer composition on performance in a supporting electrolyte
- Delineate the impact of electrolyte conductivity and alkalinity on performance and durability
- Address delamination and longer-term durability due to catalyst layer processing and reordering

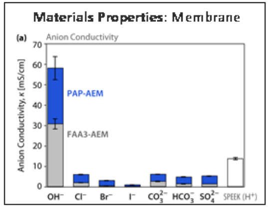
Materials Selection

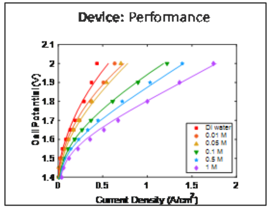
- Electronic Structure Modeling (**NREL**)
- Ionomer Thin Films (**LBNL**)
- Microelectrodes (**LBNL**)

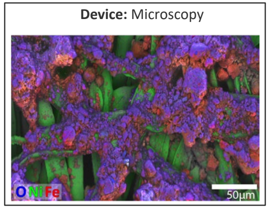
- In-situ Cell Testing (**NREL**)
- Microscopy (**SNL**)
- Multiscale Model (**LBNL**)

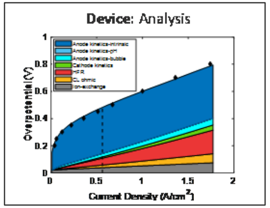
Materials → Devices







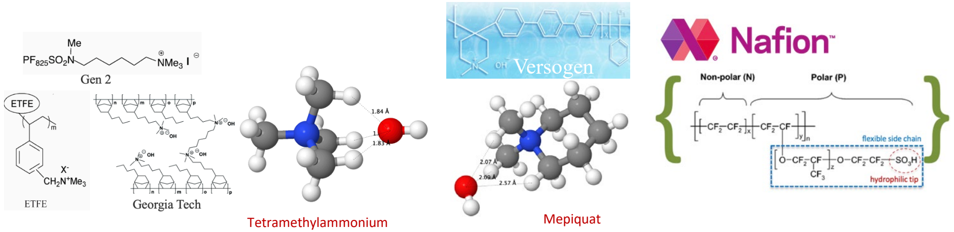




LTE Lab R&D Accomplishments:
Understanding Ionomer Effects on Oxygen Evolution

6 Nodes

Approximate Ionomer with Smaller Organic Fragments: Theoretical calculations can give critical insights into ionomer-catalyst chemistry



Ionomer-Catalyst Interactions: $N^{+}R$ group can poison activity by blocking sites, degrade, or introduce competing reactions to OER

- Does ionomer ***poison the catalyst*** by introducing competing reactions or covering sites?
- Does the ionomer ***remain stable or does it degrade*** into other species?
- Experiment-Theory Assessed Stability on **Versogen, Nafion, and Georgia Tech** Ionomers
- On model IrO_2 and NiO: Nafion's SO_3 *may be competitive or even block metal sites*

Ir-OH*	Ir-SO_3-Ir*	Ni-OH*	Ni-SO_3-Ni
E_{OH} (eV) = -3.72	E_{SO3} (eV) = -3.72	E_{OH} (eV) = -1.49	E_{SO3} (eV) = -1.97

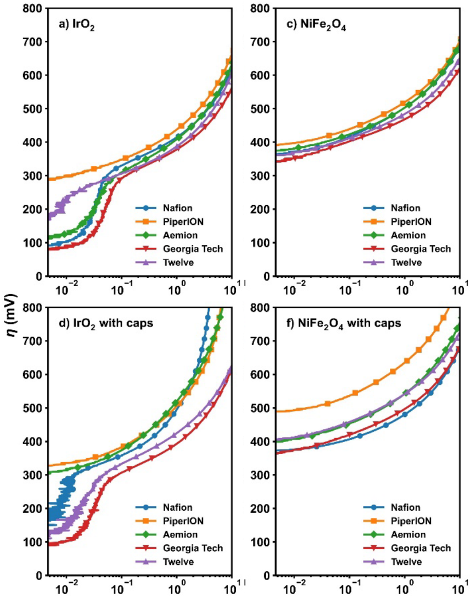
Nafion's SO_3 → *Competitive* to OH on IrO_2

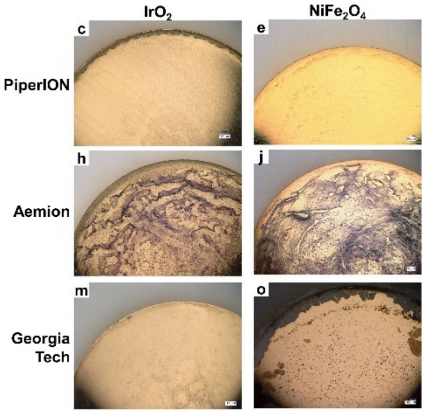
Nafion's SO_3 → *Poison* Ni Sites on NiO

Theory can identify *key limitations or advantages* to specific ionomers, critical to our understanding of the ionomer/catalyst interface

Q3 QPM: Develop a measure of ionomer fragment stability on Ni-based catalyst surfaces through ab-initio simulations for 3 ionomer types. Correlate and demonstrate consistency to their relative stability in ex-situ testing through the decrease in electrode current over ≥ 10 h.

- Differences in performance observed, particularly with high ionomer content, not fully explained by changes to surface area (estimated by the double layer capacitance)
- Cyclic voltammetry reveals possible catalyst-ionomer interactions, notably changes to and the emergence of new reduction/oxidation pairs

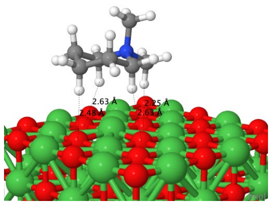




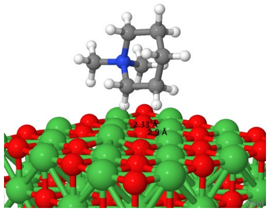
LTE Lab R&D Accomplishments:
Understanding Ionomer Effects on Oxygen Evolution's OH

6 Nodes

Versogen on NiO → *Stable,* Ni active sites available

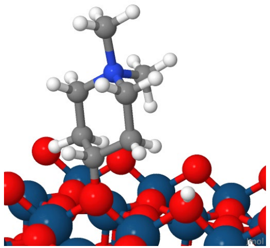


I, E_{ads} (eV) = -0.73
Stable

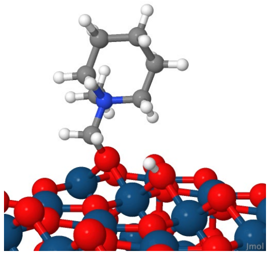


II, E_{ads} (eV) = -0.67
Stable

Versogen → *Unstable* on IrO_2

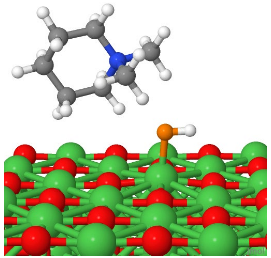


I, E_{ads} (eV) = -6.41
De-protonation

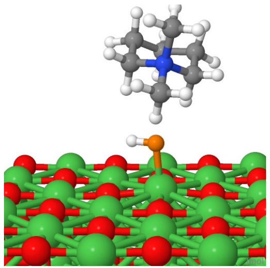


II, E_{ads} (eV) = -6.38
De-protonation

Versogen + OH* on NiO → Ni active sites available

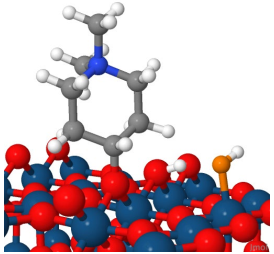


I, E_{ads} (eV) = -0.72
Water Formation

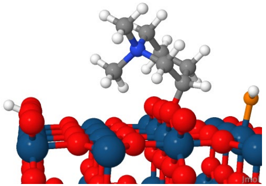


II, E_{ads} (eV) = -0.70
Methanol Formation

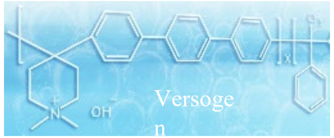
Versogen on IrO_2 → Ionomer Degrades, but OH* Adsorption Still Occurs

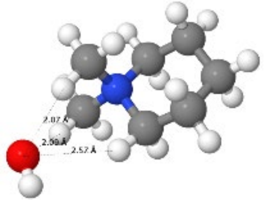


I, E_{ads} (eV) = -6.86
Co-adsorption



E_{ads} (eV) = -6.76
Co-adsorption





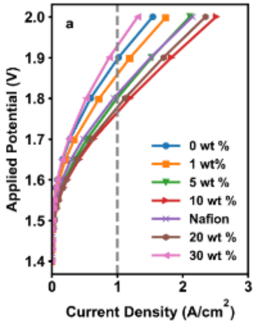
- **Versogen's** ionomer utilizes the mepiquat cation, **$C_7H_{16}N$,** to transport OH to the surface
- On **NiO**, Versogen remains stable, and metal active sites are available for OH adsorption for OER to occur
- On **IrO_2**, Versogen degrades, but still allows for OH* adsorption to occur

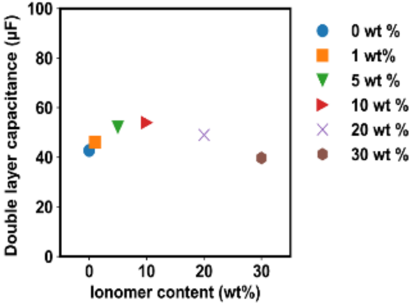
Experiment and theory assessed the stability of three ionomers (Nafion, Georgia Tech, and Versogen):

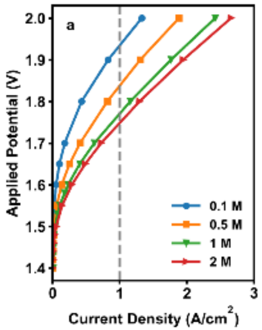
- **On NiO, IrO_2: *Versogen*** is the most advantageous, allowing for OH* adsorption for OER
- **Nafion** may adsorb too strongly, *poisoning active sites*
- **Georgia Tech** may reduce activity by *introducing competing reactions to OER*

LTE Lab R&D Accomplishments:
Understanding the Role of the Ionomer

6



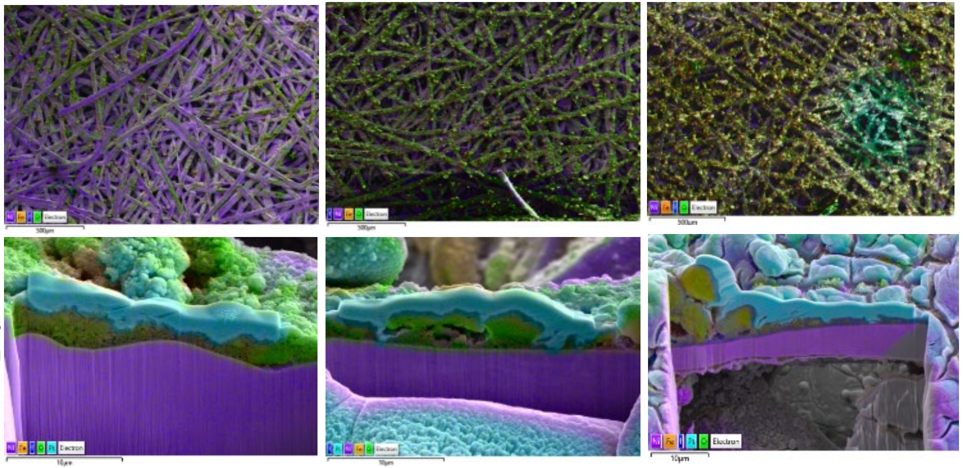




0 wt% | **5 wt%** | **30 wt%**

Top down

Cross section



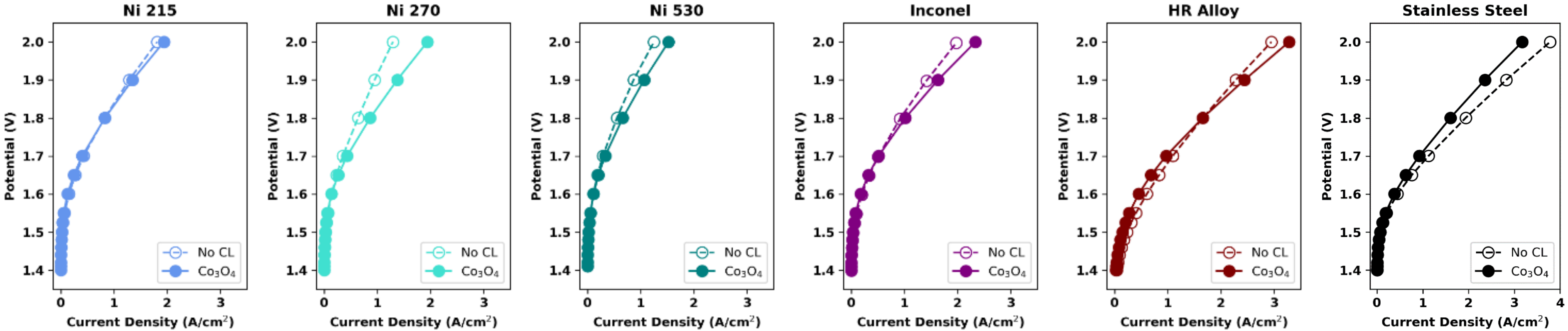
Highlight: Best performance for samples with intermediate ionomer content, associated with improved surface area and site-access. Ionomer needed for catalyst layer integrity (binder), not ion conduction.

- Performance of 10 wt% Nafion similar to 5-20 wt% Versogen, suggests that ionomer is not required for ion conduction
- Kinetic, catalyst resistance improves with electrolyte concentration, suggests that 1 M is sufficient to provide ion conduction

Achieved Q1 QPM: Correlate physical catalyst layer properties in microscopy (ionomer distribution, pore structure) to relative kinetic (Tafel and catalyst layer resistance) performance in an aqueous electrolyte for > 3 membrane electrode assemblies.

- ➢ Catalyst layer porosity increases with decreasing ionomer content. Conversely, denser and thinner catalyst layers observed for high ionomer content (30 wt%).
- ➢ Ionomer hotspots observed for 30 wt% sample – zoomed in image indicates this hotspot has dense, cracked coverage. Suggests inhomogeneity of catalyst/ionomer in the catalyst layer at high content.

LTE Lab R&D Accomplishments:
Impact of Porous Transport Layer on Performance



PTL	Composition	Thicknesss (μm)	Top Layer Fiber Dimension (μm)	Porosity (%)	Average Pore Size (μm)	HFR-free V @ 1 A/cm²	
						No CL	Co_3O_4
Ni 215	100% Ni	215	20	84	44	1.770	1.751
Ni 270	100% Ni	270	20	61	18	1.845	1.746
Ni 530	100% Ni	530	20	60	16	1.877	1.808
Inconel	60% Ni, 25% Cr, 15% Fe	600	12	65	22	1.737	1.719
HR Alloy	60% Ni, 22% Cr, 16% Mo, 2% Fe	290	4	45	7	1.591	1.632
Stainless Steel	65% Fe, 18% Cr, 14% Ni, 3% Mo	430	2	44	9	1.663	1.628

Highlight: Transport layer clearly utilized in anode reactivity, approaches 4 A cm^{-2} at 2 V without catalyst layer

- Improved activity through the addition of other elements (Fe, Cr, Mo)
- Nickel transport layers less active, likely required for long-term durability

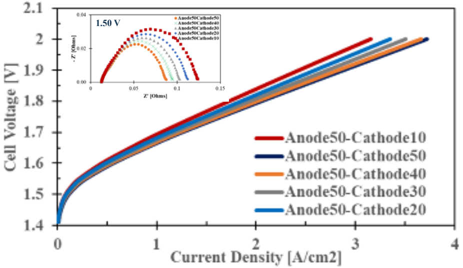
Anode: none or 0.5 mg$_{TM}$ cm^{-2} Co_3O_4 (USRM); **Cathode:** 0.3 mg$_{Pt}$/cm^2 Pt/C (TKK); **Electrolyte:** 1 M KOH; **Temperature:** 80 °C; **Membrane:** PiperION TP-85 (80 μm); **Ionomer:** PiperION TP-85 (30 wt%); **Cathode GDL:** MGL280 C paper; **Anode PTL:** Ni 18-025 (Ni) or ST10AL3 Alloy HR (HR) or XL601S AISI 316L (SS) (Bekaert)

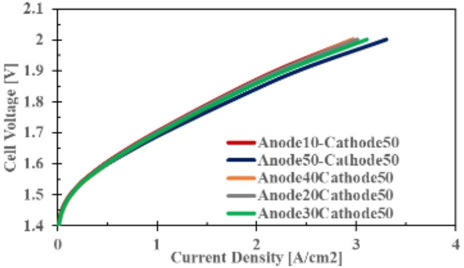
LTE Lab R&D Accomplishments:
Effect of Operational Parameters

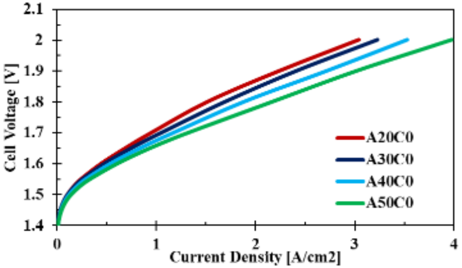
Achieved Q2 QPM: Leverage *ex* and *in* situ resistance/impedance measurements to separate sources for electronic and ionic resistance for $\geq$ 2 membrane electrode assemblies varying catalyst layer deposition approach. Correlate to modeling to demonstrate consistency in overpotential sources and compare kinetic performance (cell at 1 A cm^{-2}) and catalyst layer utilization (cell-level model) data to down select catalyst layer fabrication approach.

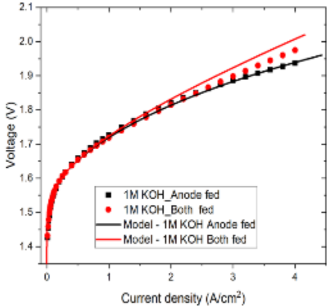
- Agreement between modeling and cell testing when incorporating different flow parameters, particularly with decreasing HFR at higher current density during dry cathode operation.

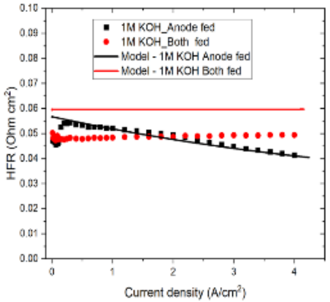
Electrolyte Flow

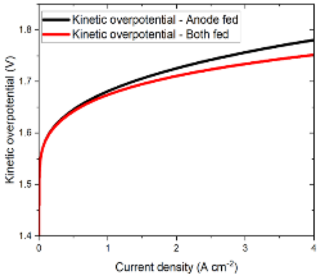


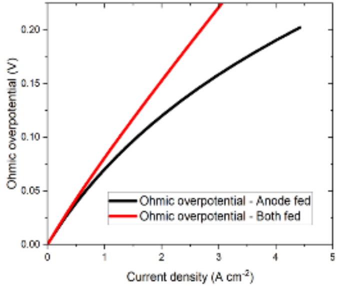








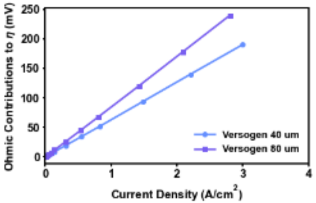


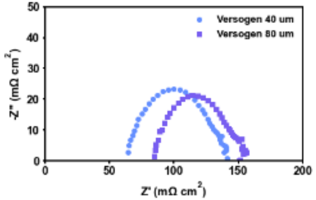


Highlight: Although feeding both anode and cathode decreases the kinetic overpotential, it has a higher ohmic overpotential

- For anode feed, the concentration gradient between anode/cathode is higher, improved mass transport
- Feeding liquid electrolyte increases bubbles entrapment

Membrane Thickness

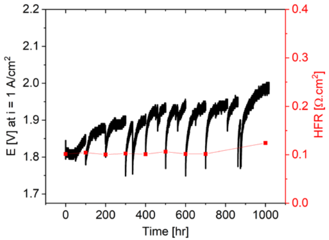


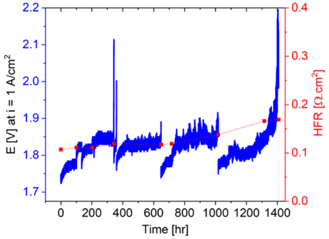


LTE Lab R&D Accomplishments:

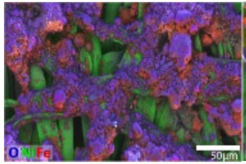
Degradation Mechanisms and Accelerated Test Development

6 Nodes

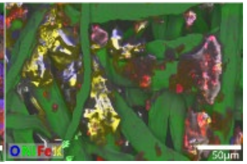




Durability at 1 A/cm^2 for MEAs with anode PTLs: (a) Ni PTL and (b) SS PTL

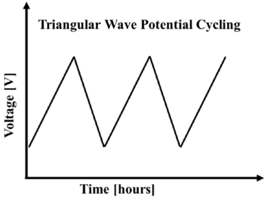


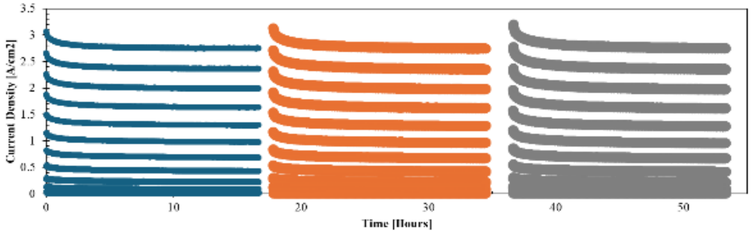
NiFe Catalyst Layer, Initial



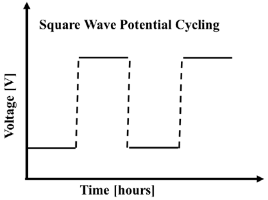
NiFe Catalyst Layer, After Test

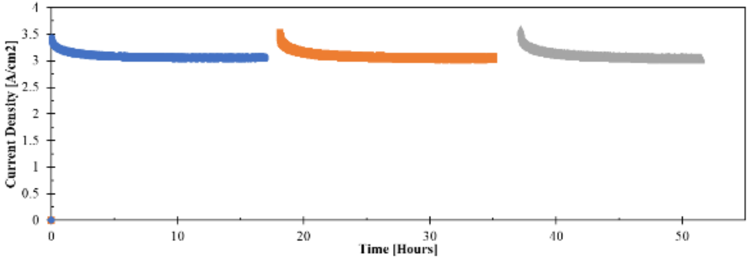
Q4 Milestone: Testing of at least 3 membrane electrode assemblies with commercial materials for at least 500 h to set a benchmark performance decay rate and understand relevant degradation processes.



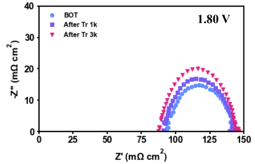


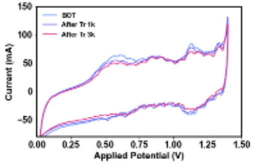
Triangle wave stability (1.45–2 V) with Co anode catalyst layer and Ni PTL

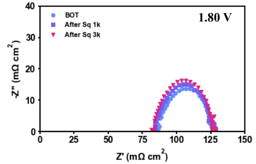


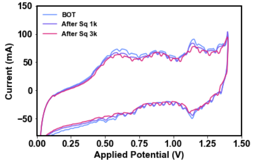


Square wave stability (1.45–2 V) with Co anode catalyst layer and Ni PTL







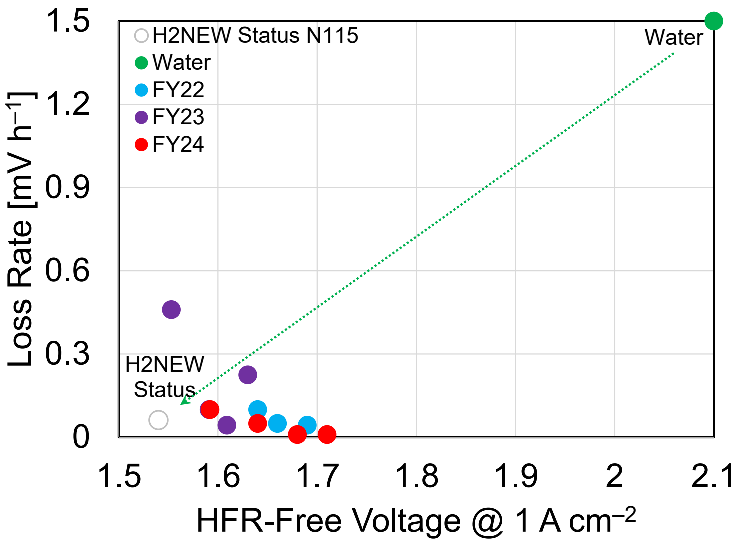


Highlight: Probing durability testing through extended operation to determine degradation mechanisms and evaluate operational strengths/vulnerabilities. Developing accelerated stress tests at the component- and cell-level.

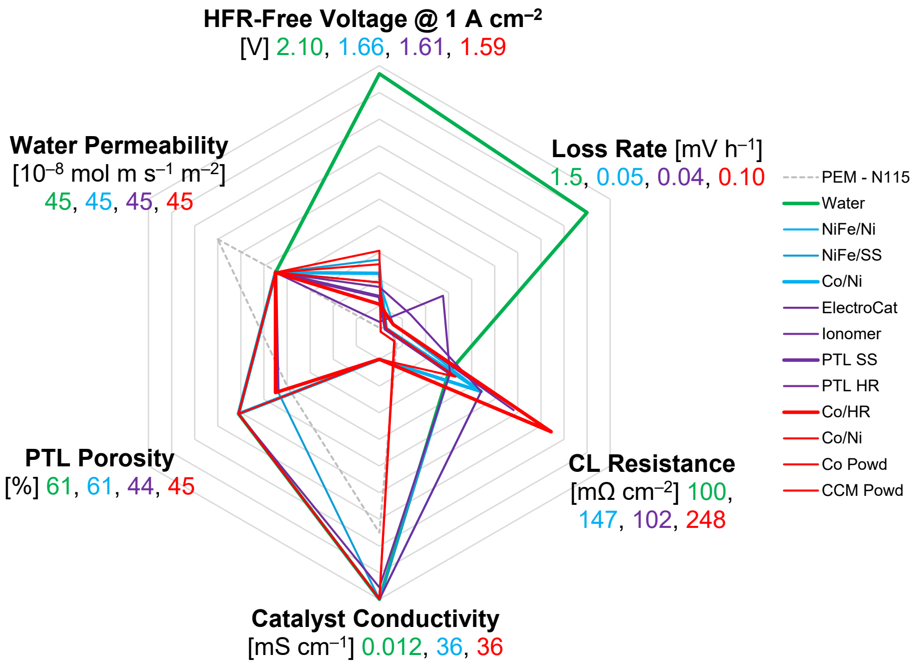
- Increased Fe mobility is a consideration. Dissolution of Fe in the catalyst layer can lead to catalyst layer delamination. Dissolution of Fe in the transport layer can lead to lower site-access and interfacial resistances.
- Short-term load fluctuation leads to a recoverable performance decrease, likely due to passivation and gas formation impacting site-access. Minimal changes in kinetics found from voltammetry and impedance.

LTE Lab R&D Accomplishments:
Overall Progress and Proposed Metrics

Proposed AEMWE Figure of Merit & Technical Progress



Proposed AEMWE Metrics



LTE Lab R&D Accomplishments Summary and Proposed Future Work

Accomplishments Summary

- Ionomer stability can range considerably depending on the catalyst material, even on the typically non-reactive model NiO and on the benchmark PGM IrO_2 with degradation introducing competing reactions to OER such as alcohol or water formation
- Established the role of the ionomer in catalyst layers and probed the impact of various ionomers on catalyst reactivity and stability, leveraging modeling to understand catalyst-ionomer interactions
- Demonstrated performance improvements through the screening of transport layers and optimization of ionomer content and ionomer integration strategies, leveraging microscopy to understand performance differences between catalyst/transport layers
- Began durability testing to establish loss mechanisms and to development component- and cell-level accelerated stress tests

Proposed Future Work

- Evaluate OH* coverage effects on ionomer stability; determine transition state barriers to oxygen evolution in the presence of the ionomer to assess changes to OER activity
- Establish an understanding of how various ionomer chemistries and catalyst compositions modify catalyst layer reactivity-stability relationships
- Optimize catalyst layer composition and processing technique to improve site-access, catalyst layer resistances, and device performance and durability
- Understand the impact of catalyst layer electronic and ionic conduction on catalyst layer resistance and cell performance
- Establish benchmark performance decay rates and understand relevant degradation processes; create durability testing framework for component- and cell-level stress tests.
- Leverage HydroGEN nodes to enable successful HydroGEN seedling and Lab Call projects

Any proposed future work is subject to change based on funding levels

High Temperature Electrolysis (HTE) Technical Accomplishments: Dong Ding

Participating Labs: INL, LBNL, LLNL, NREL

Project ID # P148B

HydroGEN HTE Seedling Projects and Lab Collaboration

Project-driven tech transfer, resulting in

- Efficiency
- Yield
- Cost
- Durability
- Manufacturability

HTE Node Labs

Idaho National Laboratory (INL)

NREL Transforming ENERGY

Sandia National Laboratories

BERKELEY LAB

Lawrence Livermore National Laboratory

Support through:

Personnel

Equipment

Expertise

Capability

Materials

Data

Interactive HTE Projects

p-SOEC

Seedling FOA projects

Raytheon Technologies

Georgia Institute of Technology

West Virginia University

The UNIVERSITY of OKLAHOMA

COLORADO SCHOOL OF MINES

Lab call projects

INL Idaho National Laboratory

Lawrence Livermore National Laboratory

o-SOEC

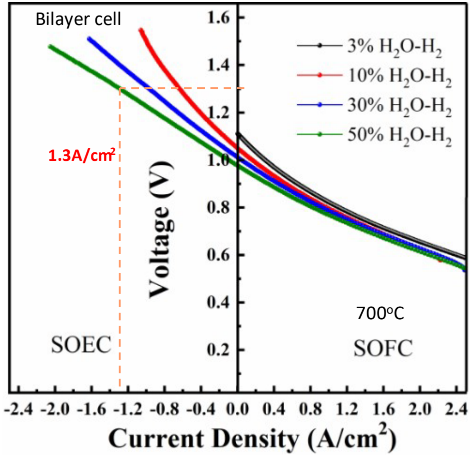
SAINT-GOBAIN

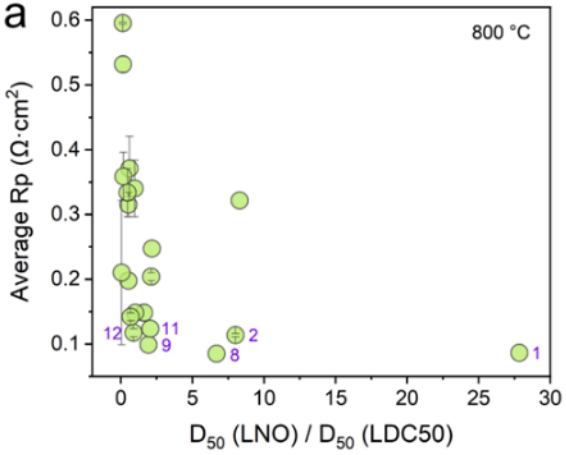
UNIVERSITY OF South Carolina

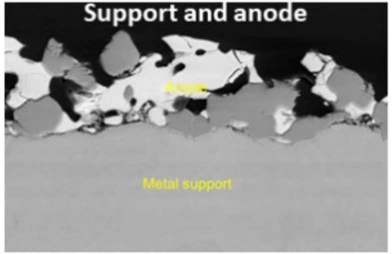
HydroGEN HTE Seedling Projects with Lab Capability Support

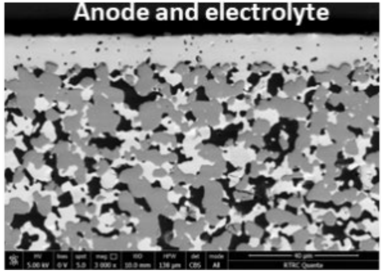
Technical Accomplishment Highlights

- **(P190, USC, INL and NREL) A Multifunctional Isostructural Bilayer Oxygen Evolution Electrode for Durable Intermediate-Temperature Electrochemical Water Splitting:** Solid oxide electrolyzer featuring a bilayer air electrode was evaluated across various H_2O-H_2 ratios. The optimal performance was observed at 50% H_2O-50% H_2, achieving 1.3 A/cm²@1.3V at 700°C.
- **(P176, Saint-Gobain and INL) Development of Durable Materials for Cost Effective Advanced Water Splitting Utilizing All Ceramic Solid Oxide Electrolyzer Stack Technology:** Symmetric cells were used to optimize the particle size ratio of Lanthanum Nickelate and Lanthanum doped Ceria, defining a working range to produce a composite air electrode with low polarization resistance and a tolerance to small batch to batch PSD variations.
- **(P154, RTRC and INL) Thin Film, Metal-supported High Performance and Durable Proton-Solid Oxide Electrolysis Cells:** p-SOEC metal cells were produced with advanced manufacturing process, showed strong bonding of metal support and electrode with no Cr diffusion at the metal-electrode interface.







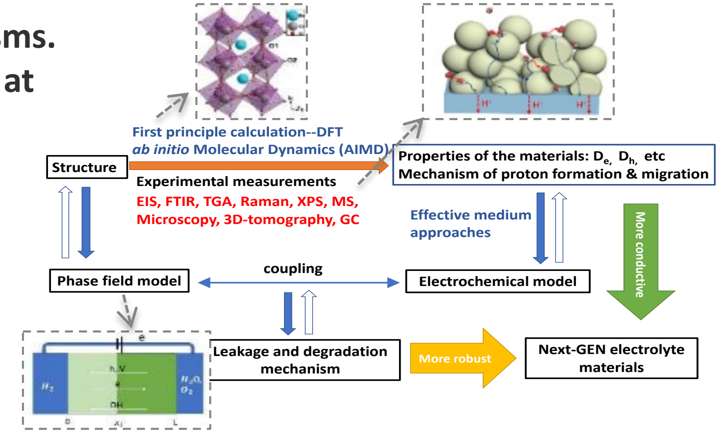


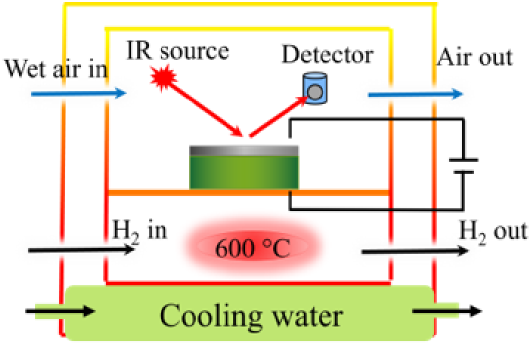
HydroGEN HTE Lab R&D p-SOEC Approach:
Combine Multi-Scale Computation and Experiment to Improve Faradaic Efficiency

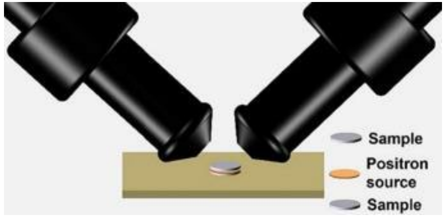
- **Develop effective approaches to suppress electronic leakage by understanding the proton conduction and electronic leakage mechanisms.**
- **Develop a robust, energy-efficient, and reliable electrolyte, for p-SOEC at 500-600°C, achieving high Faradaic efficiency (FE) and long durability.**

- **Framework:** Established an efficient framework by integrating experiment and multi-scale simulation (DFT/AIMD, phase-field model) for mechanism study in broad time and size scales.
- **Experiments:** Developed advanced characterization techniques to assess electrolytes to disclose thermodynamic information for modeling.

Mechanism study





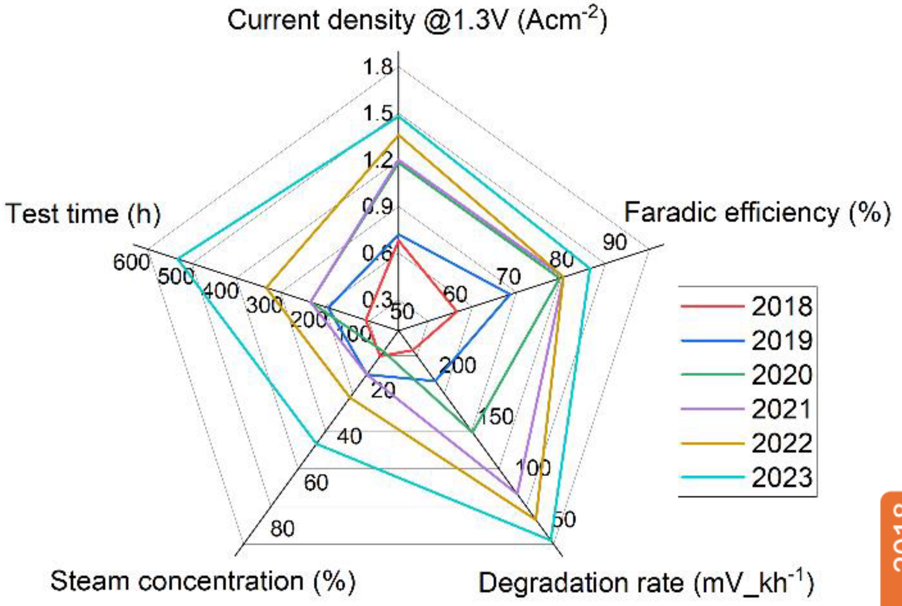


- **Electrochemical modeling:** Built framework that leverages experimental measurements, electrochemical modeling and DFT simulation to predict Faraday efficiency of p-SOECs for various of electrolyte materials.
- **DFT/AIMD:** Unraveling factors affecting the mechanical properties of electrolyte at atomic scale.

HydroGEN Lab R&D p-SOEC Technical Accomplishment:

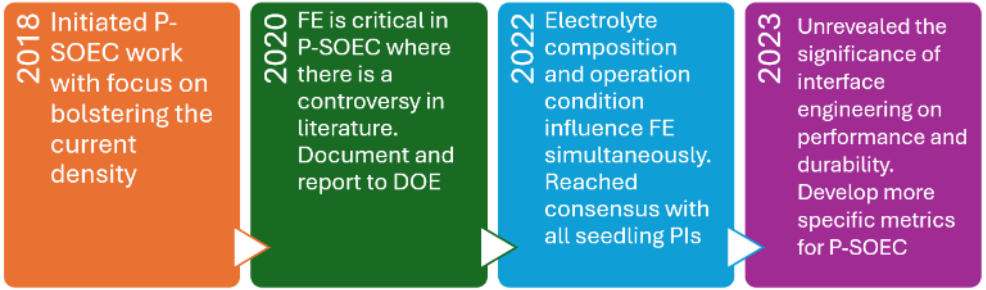
Overall Progress and Figure of Merits

INL p-SOEC Technical Progress*



- Parameters in each year represent the upper limits we achieved where test time and steam concentration are facility-constrained and have been improved significantly
- INL is focusing primarily on FE and degradation rate for a given current density and steam concentration.

- A p-SOEC metrics target table has been developed, like the one H2NEW-HTE initiated, with the additional focus on FE, FE durability and specific metrics on cell scales (e.g., button cells, single unit cells and short stack).
- As an emerging technology, technical progress and knowledge buildup are valuable to refine and reshape the technology roadmap.
- Increasing inquiries, discussions and licensing needs from industry are good signs for accelerating P-SOEC penetration to the market.



* Data derived from INL internal reports and publicly available publications

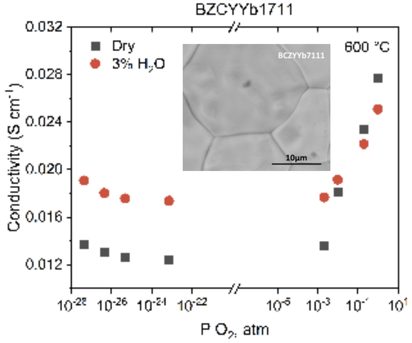
HydroGEN Lab R&D p-SOEC Technical Accomplishment:

Synergies between numerical simulations and experiments to derive Faradaic efficiency

- ✓ Conductivity of the electrolyte material determines the Faradaic efficiency for a given operation condition with some basic assumptions.

- ✓ The framework validated the experimental data from full cell testing well, and provided the FE predictions under extreme conditions

Total conductivity measurement

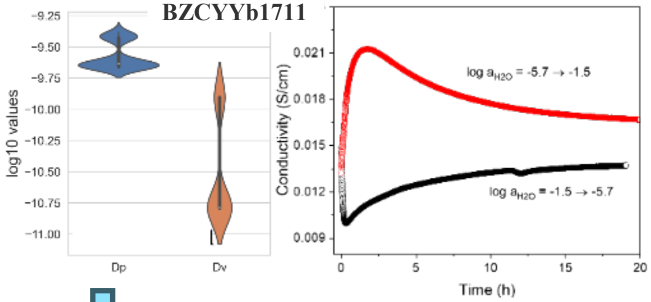


P Zhu, et al. under review

Inform

Parametric model: derive parameters

Verification: ECR experiments



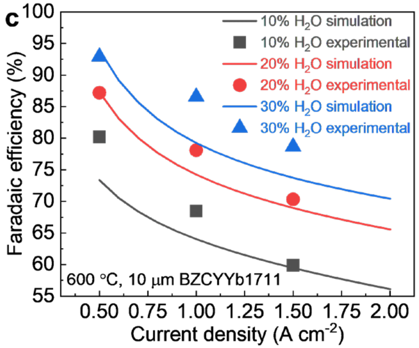
Y Meng, et al. under review

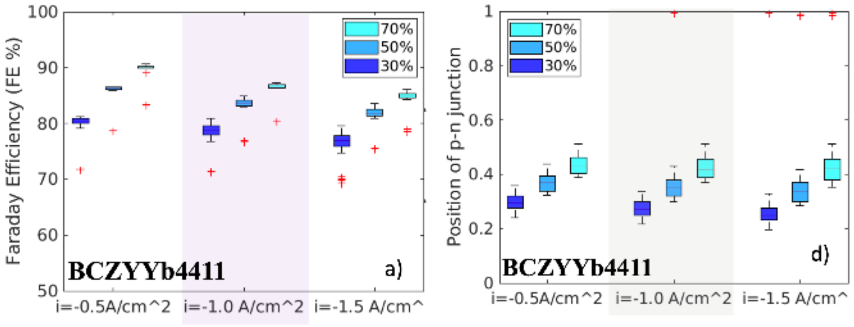
Feed-in

Validation

Experimental measurement

Electrochemical model: FE prediction





W Zhang, et al. under review

p-n junction verification: DFT simulation

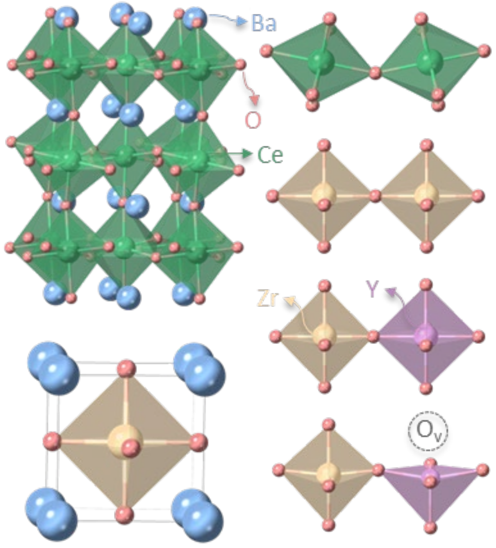
Q Zhang, et al. under review

HydroGEN Lab R&D p-SOEC Technical Accomplishment:

Factors Affecting the Mechanical Properties of Proton-Conducting Perovskite Electrolytes

- **Key compositional and microstructural factors affecting mechanical properties**
  - Composition ($BaCeO_3$ vs $BaZrO_3$)
  - Lattice phase (Cubic vs. Orthorhombic)
  - Defect (O_v)
  - Octahedron (w/wo distortion)

- **Mechanical properties from first-principles calculations at atomic scale**
  - Doping and defects create elastic anisotropy and orientation-dependent elastic moduli, which may cause anisotropic fracture propagation and thermal expansion.
  - Reducing lattice symmetry decreases elastic moduli, increasing susceptibility to failure under cycling.

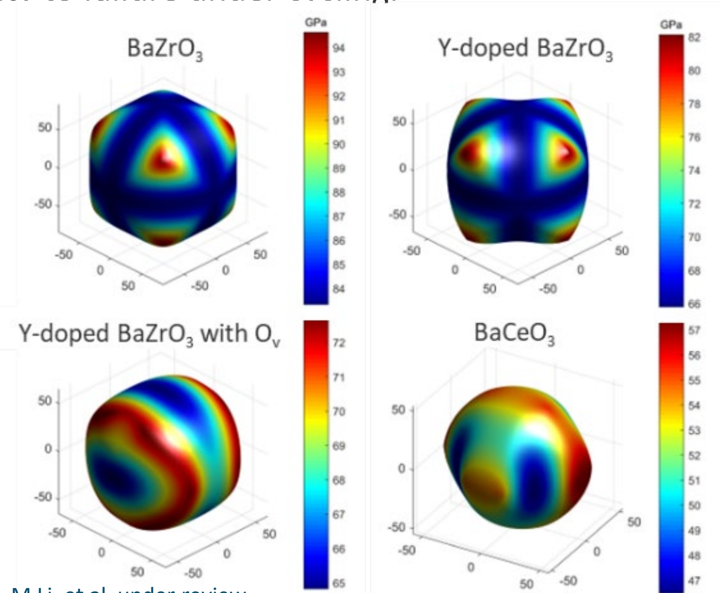


Composition / Structure

Mechanical properties

Insights on mechanical properties at atomic scale:

- Deformation
- Fracture behavior
- Fatigue resistance
- Thermal expansion

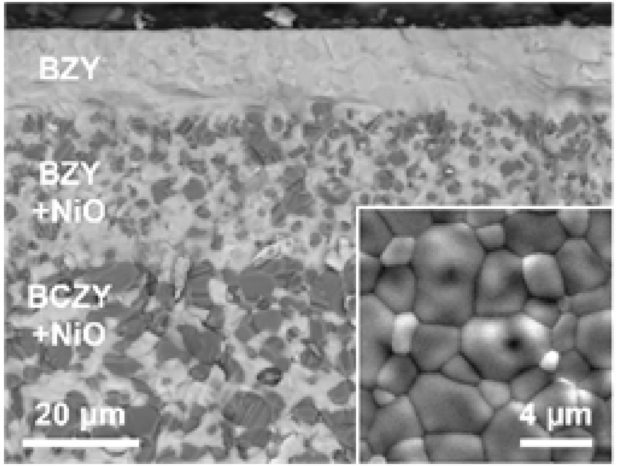


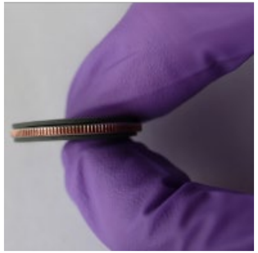
M Li, et al. under review

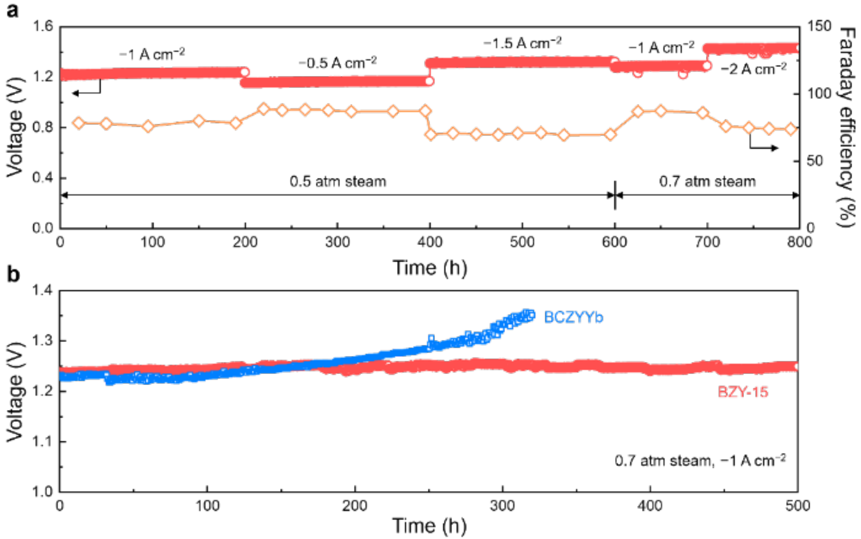
HydroGEN Lab R&D p-SOEC Technical Accomplishment:
Benchmarked BZY cells with enhanced electrolysis stability and Faradaic efficiency

Performance and durability of p-SOEC is equally important for its advancement and adoption by the market.

- Additional effort is placed on the full cell durability, especially under some extreme conditions.
  - Benchmarked electrolyte BZY is employed
  - Cells successfully underwent different current densities (up to 2 A cm^{-2}) and steam concentrations (up to 70%)
- New fabrication methods suppressed Ce effect on electrolyte and enabled the flat cells with clean grains.
- The Faradaic efficiency can be maintained at ~ 90% at −1 A cm^{-2} with 70% stream concentration at 600°C with a durable operation (single condition >500 hrs and multi-conditions > 800 hrs). Combined with the modeling prediction conducted under 99% steam concentration, it suggested the **completion of the annual milestone (FE >95% and tested for 500 hrs)**







W Tang, et al. under review

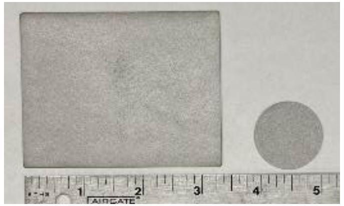
HydroGEN HTE Lab R&D Technical Accomplishment:
LBNL Metal-Supported Solid Oxide Electrolysis Cell (MS-SOEC)

Project targets at 700°C, 50:50 H_2O:H_2

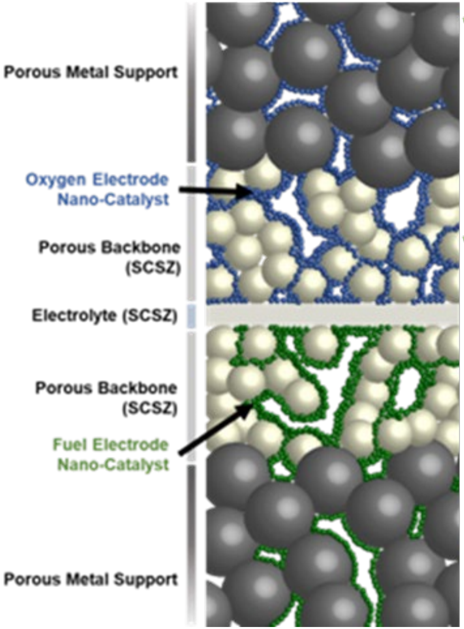
<u>Cell size (complete)</u>
Target: >40 cm^2
FY24 Status: 50 cm^2

<u>Performance (complete)</u>
Target: > 1.0 A/cm^2 at 1.4V
FY24 Status: 1.3 A/cm^2 at 1.4V

<u>Durability (ongoing)</u>
Target: <5%/kh
FY24 Status: 13%/kh at 0.5 A/cm^2



Approaches to improve performance and durability



Protective coatings to block Cr
- Particle size
- Composition
- EPD deposition parameters
- Sintering protocol

Catalyst composition and processing
- Alternative OER catalysts
- Coatings to prevent LSCF-ScSZ reaction
- Micron-scale Ni to prevent coarsening

Cell structure and processing
- Processing in air to allow high-T sintering of catalysts

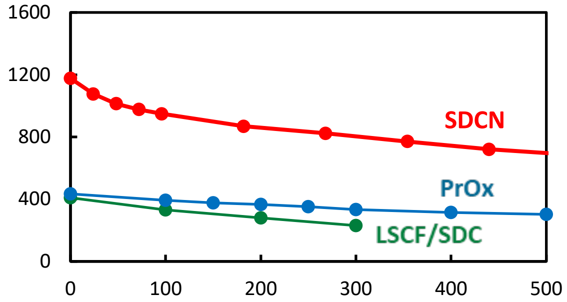
Diagnostics and model cells
- Symmetric cells to isolate each electrode
- Cr dosing
- Pre-oxidize metal support
- Refresh catalyst after long-term operation
- Post-mortem at 0, 100, 300, 1000h

MS-SOEC Model cells to assess degradation modes

LBNL HTE Lab R&D Accomplishments

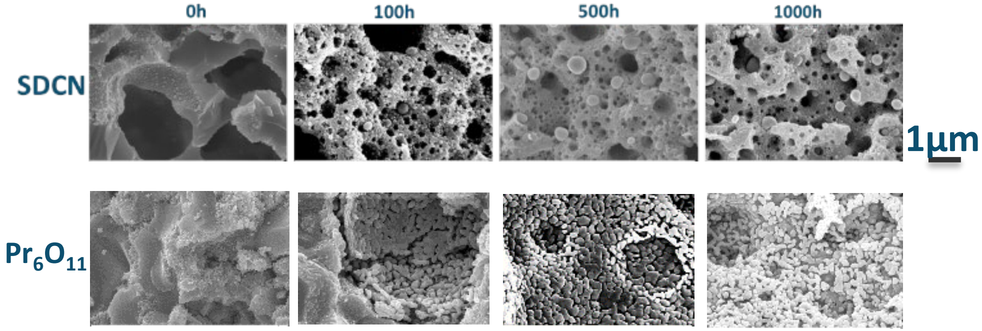
Symmetric cells

Oxygen catalysts dominate: lower performance and durability than SDCN



Detailed post-mortem analysis

Separating break-in and long-term degradation phenomena

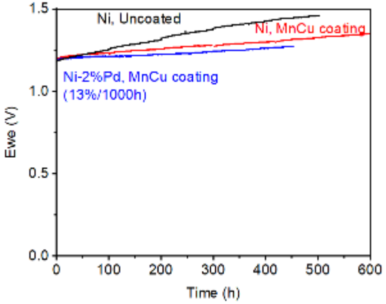


Ni alloy

2% Pd doping increases stability

- suggests less expensive alloys may be fruitful

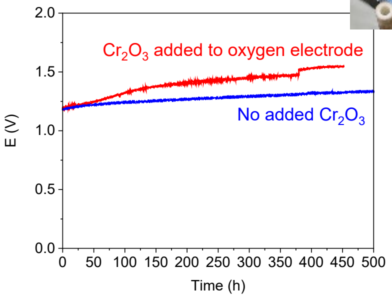
MnCu coating on air-side stainless steel support reduces Cr migration



AST: Cr Dosing

Adding Cr accelerates degradation

- Saturates in ~150h



Conclusions

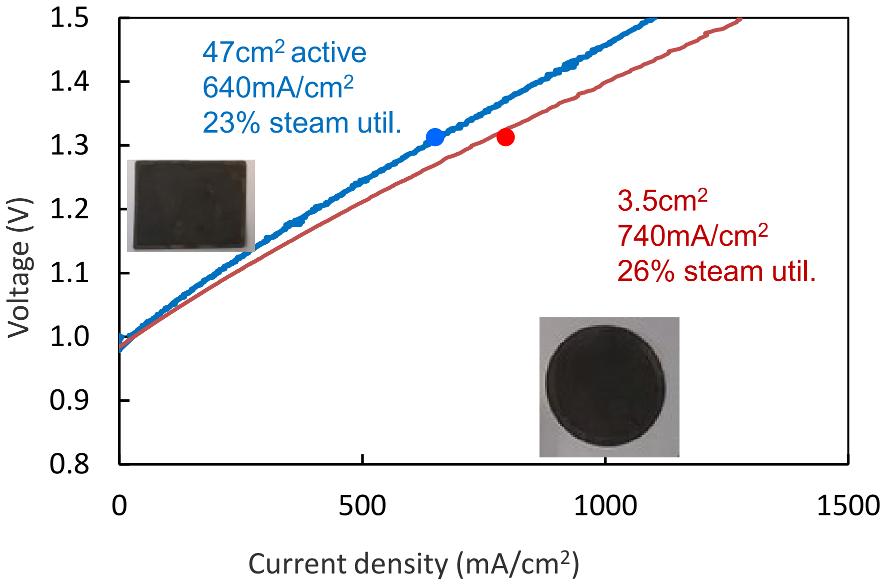
- Oxygen electrode limits performance and durability
  - Cr poisoning is significant in SOEC mode
- Ni coarsening is complete at <500h
- PrOx coarsening is complete at 100h
- SDC coarsening is minor

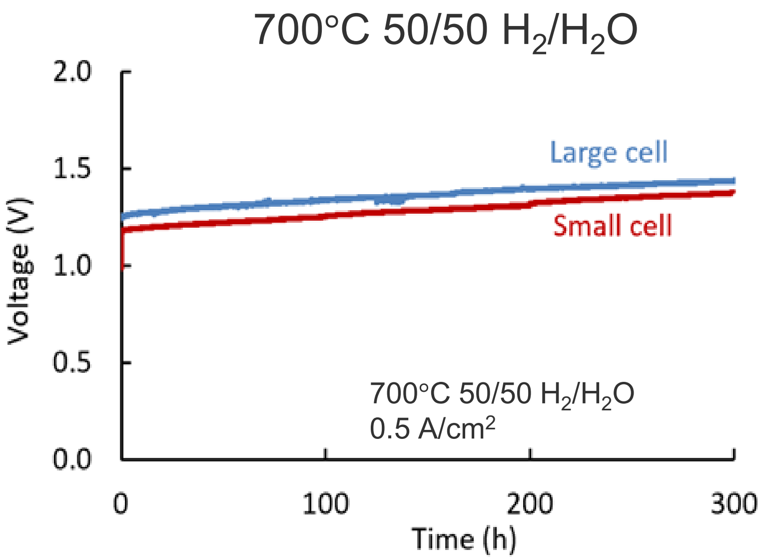
Priorities

- Cr-blocking coating
- Increase Ni and LSCF/Pr particle size
- Alternative to infiltrated catalysts
  - Ni alloy or exsolution
  - conventional OER catalyst

MS-SOEC Scale-up to 50 cm^2 cell size

LBNL HTE Lab R&D Accomplishments

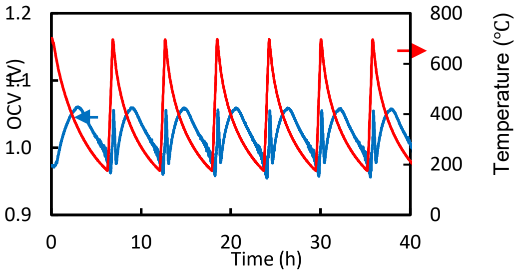


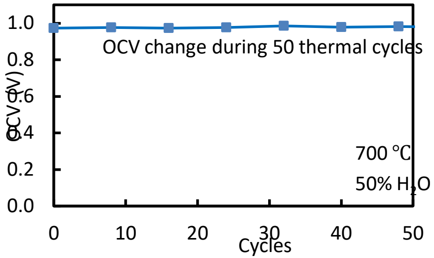


- Good performance for large planar cell
- Performance and durability are similar to button cell
  - **86% of button cell current density at 1.3V (exceeds target of 75%)**

MS-SOEC Dynamic Operation at 700°C
LBNL HTE Lab R&D Accomplishments

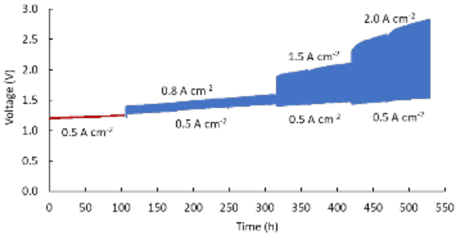
Thermal Cycling

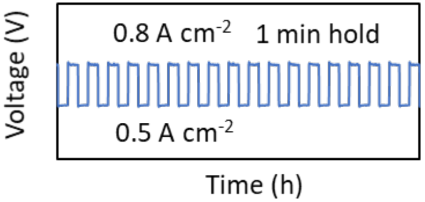




50 cycles from
160°C to 700 °C

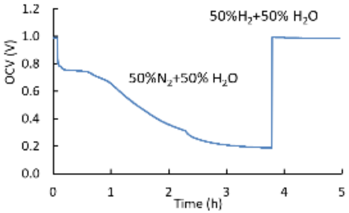
Current Cycling

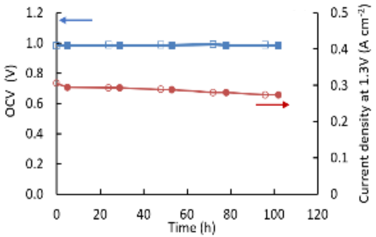




13,500 cycles between
0.5 A/cm² and 0.8-2 A/cm²

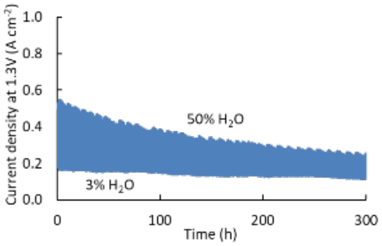
Redox Cycling

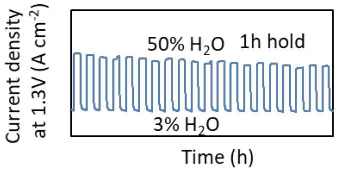




5 cycles from
Ni to NiO

Steam Content Cycling





150 cycles from
3% to 50% H_2O:H_2 ratio

MS-SOEC tolerates aggressive dynamic operation conditions
First report of MS-SOEC dynamic operation

HTE Accomplishments Summary and Suggested Future Work

Accomplishments Summary

- **Lab capability support:** Effective collaborations between the seedling projects and the lab nodes, significantly accelerating both o- and p-SOEC technology advancement.
- **p-SOEC Lab R&D**: Investigated the fundamentals of protonic ceramic electrolytes and emphasized equal importance in performance and stability of p-SOEC with improved Faradaic efficiency, based upon the benchmarked electrolyte materials.
- **MS-SOEC Lab R&D** : Demonstrated robustness of MS-SOEC to dynamic operation; scale-up to cell size 50 cm^2; systematic analysis of degradation phenomena; screening of concepts to improve durability.

Proposed Future Work

- Continue leveraging the lab node support for the upcoming FOA projects.
- Benchmark and develop the p-SOEC electrolyte materials that have higher proton conductivity, better stability, less electronic leakage, and better chemo-mechanical properties.
- Develop MS-SOEC with further improved durability; Develop alternative cell architecture and fabrication approaches

Any proposed future work is subject to change based on funding levels

Photoelectrochemical Water Splitting (PEC): Joel W. Ager

Participating Labs: LBNL, NREL, LLNL

- Todd Deutsch (NREL)
- Myles Steiner (NREL)
- James Young (NREL)
- Julia Lenef (NREL)
- Kiseok Oh (NREL)
- Francesca Toma (LBNL)
- Peng Peng (LBNL)
- Olivia Alley(LBNL)
- Tadashi Ogitsu (LLNL)

Project ID # P148C

HydroGEN PEC Seedling Projects & Lab Collaboration

PEC Node Labs

NREL Transforming ENERGY

BERKELEY LAB

Lawrence Livermore National Laboratory

Support through:

Personnel

Equipment

Expertise/Protocols

Capability

Materials/cells

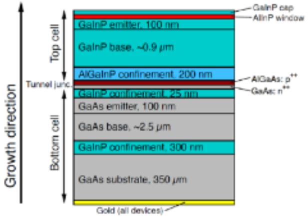
Data

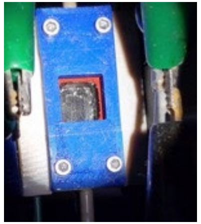
Interactive PEC projects

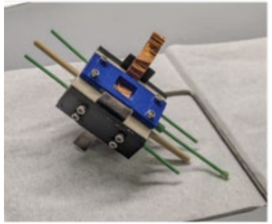
RICE

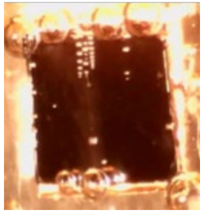
THE UNIVERSITY OF TOLEDO

UNIVERSITY OF MICHIGAN







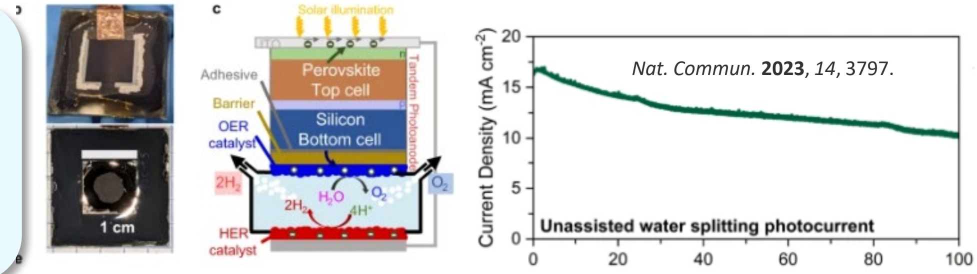


HydroGEN PEC Seedling Projects with Lab Capability Support

Technical Accomplishment Highlights

LBNL and NREL worked with **Rice University** (Aditya Mohite, P216) to characterize halide perovskite photoelectrodes coated with catalysts and a hydrophobic graphene-based barrier which ensures optimal charge transfer at the light absorber/catalyst interface.

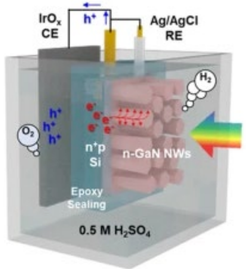
- >100 hours stability with peak efficiency >20% STH.



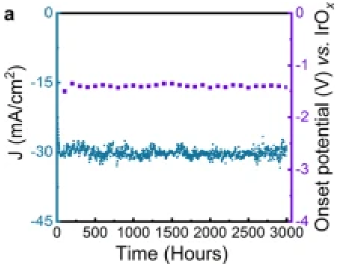
Nat. Commun. **2023**, *14*, 3797.

LBNL and NREL worked with **the University of Michigan** (Zetian Mi, P209) to stable operation of a photocathode comprising Si and GaN, the two most produced semiconductors in the world,

- Operation for 3,000 hours without any performance degradation in two-electrode configurations.

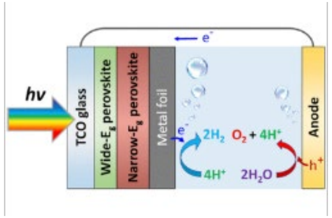


Nat. Commun. **2023**, *14*, 2047.

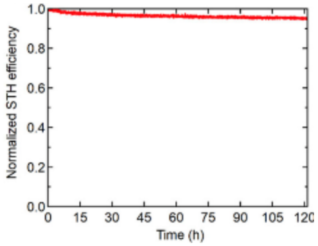


NREL worked with the **University of Toledo** (Yanfa Yan, P218) to monolithically integrate all-perovskite tandem photocathodes for unassisted solar water splitting with 15% STH.

- Continuous operation in water for >120 h at 1 sun



ACS Energy Lett. **2023**, *8*, 2611.



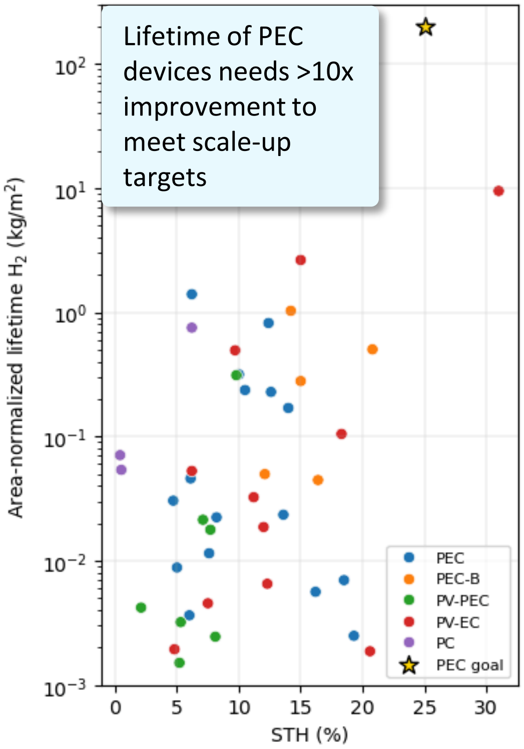
HydroGEN PEC Lab R&D Goal and Approach

STH efficiency has improved but durability has not and is limiting PEC advancement

Goal: Elucidate the degradation mechanism(s) and improve the durability of PEC materials and devices.

Approach:

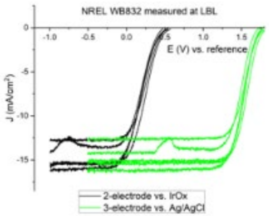
- Prioritize durability stressors and establish PEC device durability protocol
- Use density functional theory (DFT) and microkinetic modeling to describe the local environment at the electrode/electrolyte interface under operation
- Provide mechanistic understanding of PEC device degradation guided by theory and in operando characterization

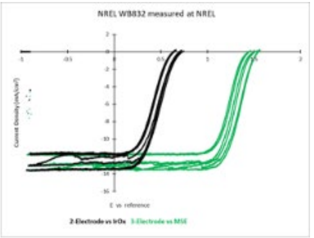


Comparison of the solar to hydrogen efficiency (STH) and lifetime H2 produced for unassisted water splitting devices. The "PEC Goal" point in the upper right. Data sourced with permission from Cheng et al. in 2022 Solar Fuels Roadmap, *J. Phys. D. Appl. Phys*. **2022**, 55 323003. PEC goal from Ben-Naim et al., *ACS Energy Lett.* **2020**, 5, 2631–2640.

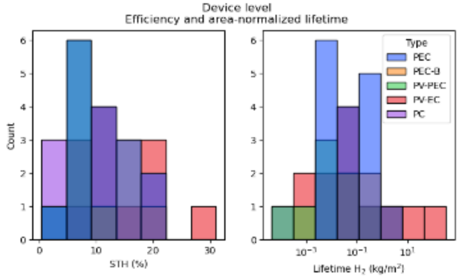
HydroGEN PEC Lab R&D Relevance and *Potential Impact*

- Develop standardized PEC device measurement techniques
  Improves reproducibility between labs

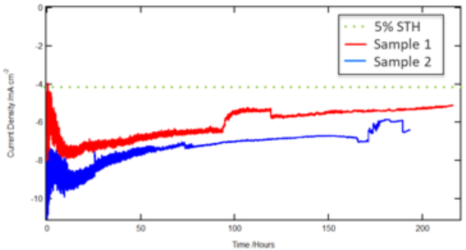




- Develop device and system-level performance metrics
  Clearly define improvements needed for economic viability

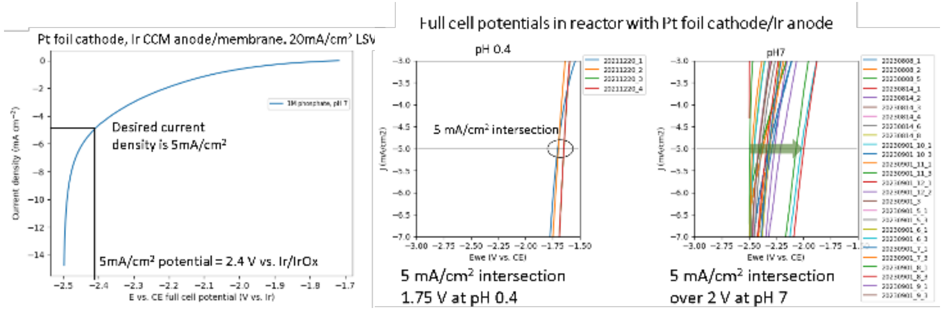


- Develop reliability science needed for closing the durability gap
  New materials for durable PEC water-splitting devices
  Accelerated wear protocols to quantify progress

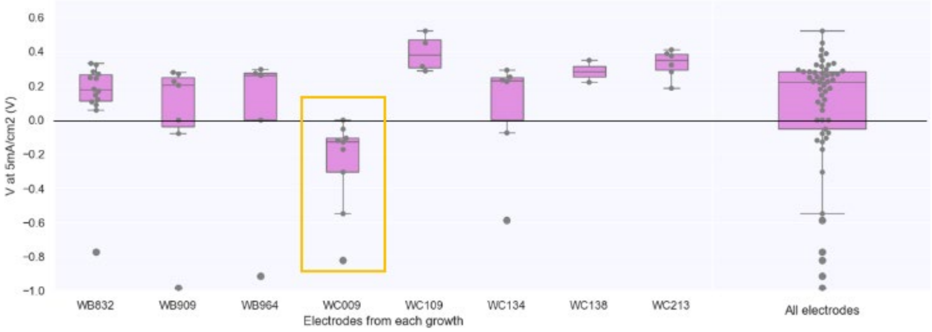


Rigorous analysis of PEC reproducibility
PEC Lab R&D Accomplishment

NREL and LBNL quantified within- vs between- growth variations for eight MOVPE photocathodes



Left: Determination of the 5mA/cm2 potential from the initial linear sweep voltammetry (LSV) scan. Center: four LSV curves from measurements done in 0.5M H2SO4 (pH 0.4), showing an approximate potential of -1.75 V. Right: 26 LSV curves from pH 7.0 measurements, including from long-path and short-path configurations of the reactor. Decreasing the path length and additional optimizations led to ~0.5 V decrease in the full cell potential.



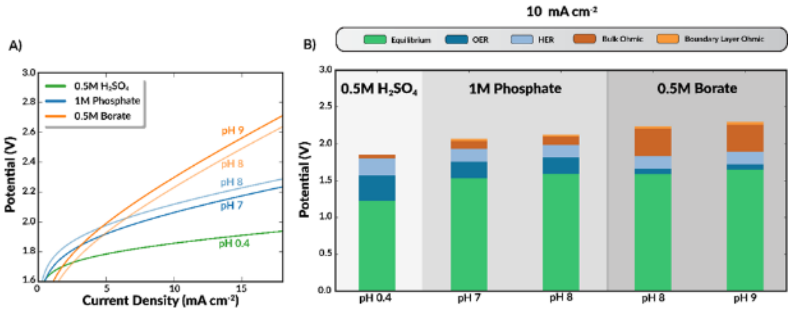
V_onset is the potential difference between working electrode (WE) and counter electrode (CE) under simulated 1 sun illumination (2 electrode measurements, 0.5 M H2SO4, pH 0.4, CE is IrOx, ca. 1 cm2, WE is PEC cell, ca. 0.2 cm2). A positive value predicts that bias-free operation is possible in acid at minimum 5 mA cm2. 67% of the runs have a positive value and there are 5 statistical outliers.

We recommend that similar statistical methods be used for comparing the initial performance and durability of different groups of PEC devices (i.e., t-tests for pairs of conditions, ANOVA multiple comparisons).

NREL and LBNL defined optimal conditions for neutral pH operation

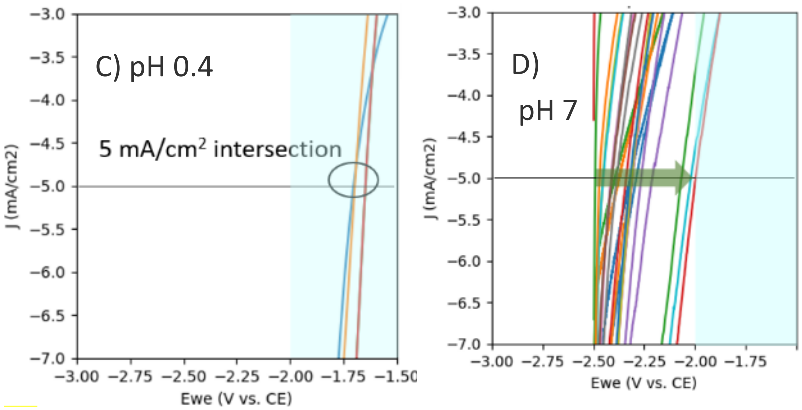
PEC Lab R&D Accomplishment

Modeling and Simulation

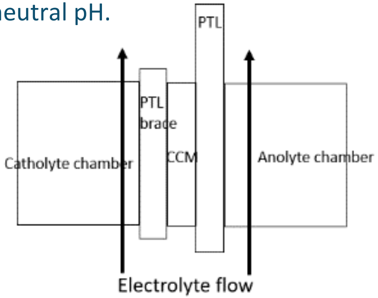


A) Polarization curves of the PEC cell with 0.5M H_2SO_4 (pH 0.4), 1M phosphate (pH 7 and 8), and 0.5 M borate (pH 8 and 9) electrolytes. B) Breakdown of contributions to voltage at average hydrogen evolution reaction (HER) current density for all the electrolytes tested at electrolyte flow rate. 0.5 M H_2SO_4 exhibits the lowest ohmic losses, but large kinetic losses. 0.5 M Borate at pH 8 has the highest ohmic losses, but the lowest kinetic potential losses.

Experiment



C) Cells operating in acid require a full cell voltage < 2 V, which is lower than the expected output of employed tandem solar cells. D) Use of catalyst-coupled membrane (CCM, schematic below) reduces required potential for 5 mA cm^{-2} operation to close to 2 V in neutral pH.



Neutral pH operation below 2 V is possible if ohmic losses are reduced

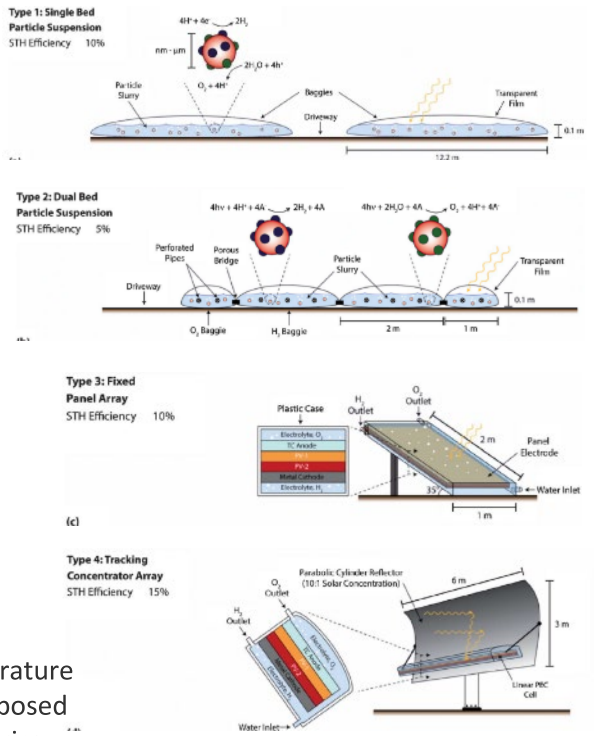
Proposed device- and system-level performance metrics
PEC Lab R&D Accomplishment

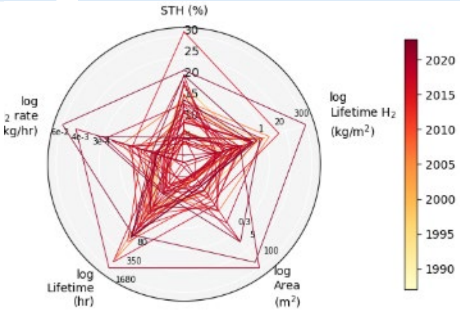
Device-level metrics

- Solar to hydrogen conversion efficiency
  STH (%)
- Area-normalized lifetime production of H_2
  kg/m^2
  normalized to PV area for concentrators

System-level metrics

- Area
  m^2
  receiver area for concentrators
- Lifetime
  hours
  as reported by source
- System H_2 production rate kg/hr





Analysis of 44 literature reports using proposed performance metrics

Parkinson, B. *Acc. Chem. Res.* **1984**, *17*, 431–437

Pinaud et al, Energy Env. Sci. **2013**.

Ager, J. W.; Shaner, M. R.; Walczak, K. A.; Sharp, I. D.; Ardo, S. *Energy Environ. Sci.* **2015**

Ben-Naim, M.; Britto, R. J.; Aldridge, C. W.; Mow, R.; Steiner, M. A.; Nielander, A. C.; King, L. A.; Friedman, D. J.; Deutsch, T. G.; Young, J. L.; Jaramillo, T. F. *ACS Energy Lett.* **2020**,

Cheng, W.-H., Deutsch, T. G., Xiang, X. in 2022 Solar Fuels Roadmap, *J. Phys. D. Appl. Phys.* 2022

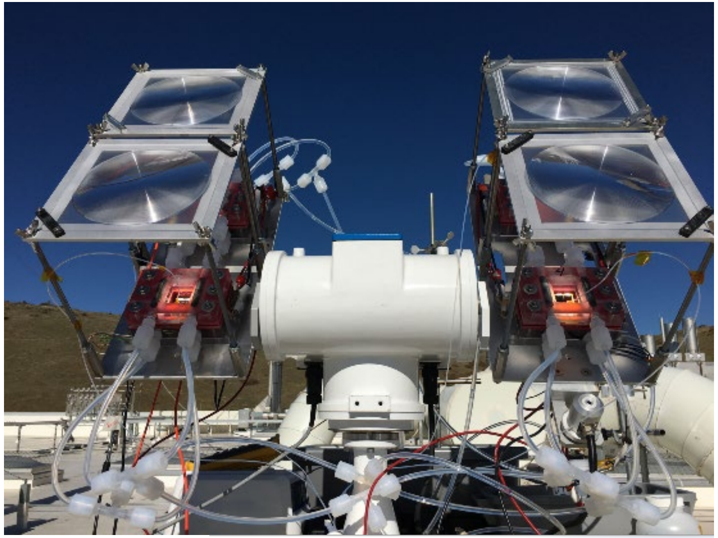
Holmes-Gentle, I.; Tembhurne, S.; Suter, C.; Haussener, S. *Nat. Energy* **2023**

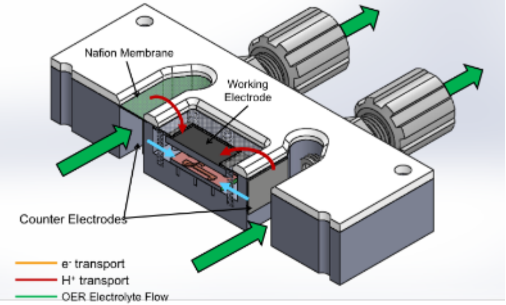
HydroGEN PEC Lab R&D Accomplishment – NREL

- **Led a breakout session at the September AWSM benchmarking workshop that focused on**
  - NREL's experience and challenges with outdoor photoreactor testing
  - Synergies among the six new awarded PEC seedling projects

- **Developed comprehensive questionnaire to assist PEC seedling projects with photoreactor setup, evaluation of device performance, and logistical considerations**
  - All seedling projects will be performing on-sun testing at NREL for 2 weeks
  - Seedling final deliverable should produce 0.1 g H_2/h (approximately 200 cm^2)
  - Testbed will be instrumented to monitor and record solar-to-hydrogen efficiency

- **Provided seedlings materials as well as characterization support and contributed to publications**
  - Rutgers: "TiO2/TiN bifunctional interface enables integration of Ni5P4 electro-catalyst with III-V tandem photoabsorber for stable solar-driven water splitting" Hwang…Dismukes et al., ACS Energy Lett. 2024, 9, 789−797.
  - Rice: "Technoeconomic model and pathway to <$2/kg green hydrogen using integrated halide perovskite photoelectrochemical cells" Fehr…Mohite et al., ACS Energy Lett. 2023, 8, 4976−4983.





PEC Accomplishments Summary and Proposed Future Work

Summary:

- Used previously developed protocols for robust benchmarking and statistical analysis of stand-alone PEC water splitting devices. (NREL/LBNL)
- Developed initial set of performance metrics for PEC devices and systems. (LBNL/NREL/LLNL)
- Demonstrated bias-free water splitting with a III-V photocathode at over 5% STH efficiency for more than 200 hours at neutral pH (NREL/LBNL)
- 7 publications

Proposed Future Work:

- Achieve FY2024 annual milestone: Stand-alone solar water splitting device of at least 4 cm^2 illuminated area capable of indoor and outdoor operation with neutral (pH ~ 7) water
- End of project goal in FY2026: Photoreactor capable of indoor or outdoor operation accommodating illuminated areas of up to 200 cm^2. Reactor will be instrumented to measure the H_2 generation rate and, optionally, to accommodate diagnostic tests meant to assess and predict durability
- Leadership in PEC community: develop and publicize device and system-level performance metrics required for PEC water splitting to meet DOE cost targets
- Leverage HydroGEN nodes to enable successful completion of current and new seedling projects

Any proposed future work is subject to change based on funding levels

Solar Thermochemical Water Splitting (STCH): Tony McDaniel

Participating Labs: SNL, NREL, LLNL, INL

Presented by: Sean Bishop

Project ID # P148D

HydroGEN STCH Seedling Projects & Lab Collaboration

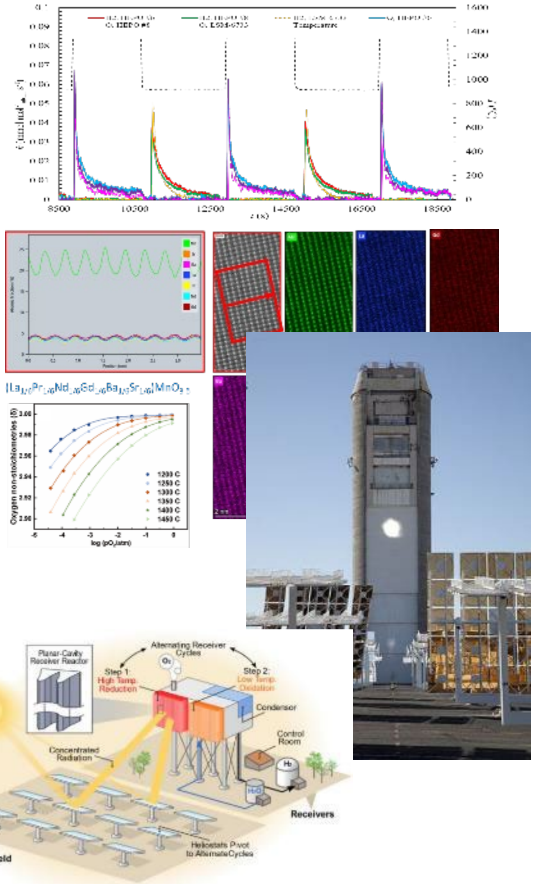
Barriers
- Cost
- Efficiency
- Durability

HydroGEN STCH Seedling Projects with Lab Capability Support

Technical Accomplishment Highlights

10 Lab capabilities support 5 new FOA-awarded projects:

- **(P211, ASU, SNL, INL and NREL) Design of Perovskite Materials for Solar Thermochemical Hydrogen Production:** Initial multiscale modeling of STCH redox reactors with comprehensive thermal-chemical models predicting component design and performance
- **(P208, CU, NREL) Non-Intermittent, Solar-Thermal Processing to Split Water Continuously via a Near-Isothermal, Pressure-Swing Redox Cycle:** Preliminary multiscale modeling evaluating STCH materials for commercial scale-up with TEA assessment
- **(P210, CU, SNL and NREL) Accelerated Discovery and Development of Perovskites for Solar Thermochemical Hydrogen Production:** Identified path forward to on-sun testing using prior reactor development.
- **(P217, St. Gobain, SNL, LLNL, and NREL) Scalable Solar Fuels Production in A Reactor Train System by Thermochemical Redox Cycling of Novel Nonstoichiometric Perovskites:** Computed energy barriers for water splitting process on STM and performed preliminary analysis of on-sun reactor testing
- **(P212, WASHU, SNL and NREL) Ca-Ce-Ti-Mn-O-Based Perovskites for Two-Step Solar Thermochemical Hydrogen Production Cycles:** Performed initial evaluation of balance of plant needs for on-sun testing.



10.1016/j.renene.2022.03.108

Assess Technology Viability, Enable DFT-ML Material Discovery
STCH Lab R&D Goals and Approach

6 Nodes

Goals: Comprehensively validate known STCH material properties and demonstrate theory-guided design of materials approach that optimizes the capacity/yield tradeoff.

- Develop computational toolset to define and establish material performance targets.
- Rigorously assess selected material formulations.
- Develop a materials search strategy for optimizing the capacity/yield tradeoff using DFT + Machine Learning (ML).
- Discover new materials using the ML model and characterize by detailed calculations, synthesis, and experimental validation.

STCH R&D:Q4 Annual Milestone	STCH Material Down-Select. Criteria: Use the technology assessment methodology derived from FY23 work to critically assess new ML-based solid solution STCH materials. The metric accounts for material-specific cycle dynamics and plant operational modality. (~10 new solid solution materials).

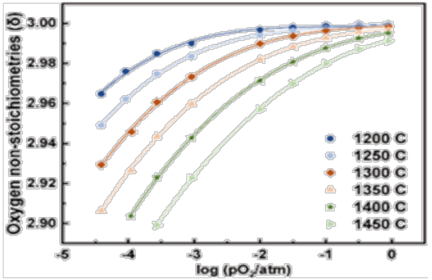
DFT = density functional theory
T_{RED} = reduction temperature

Exemplar Material Commercial Viability Study
STCH Lab R&D Accomplishments

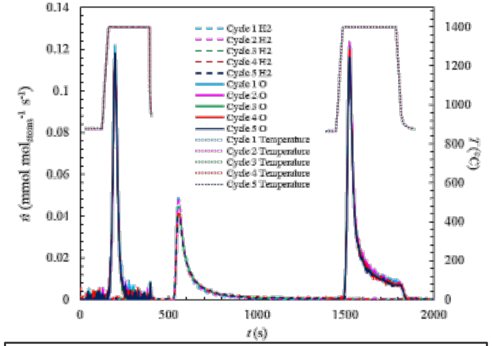
- Exemplar materials, methods and metrics determined by community consensus (via Benchmarking).
- Software platform developed for "end to end" processing of experimental data.
  - Will be made available to public

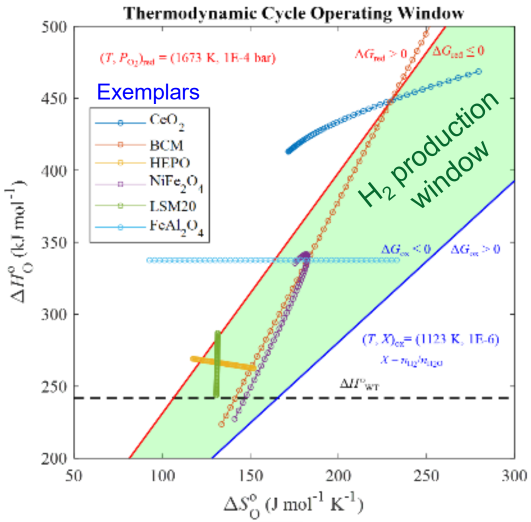
Key accomplishment: Measured and analyzed thermodynamics and H_2 production of five exemplar materials
Next step: Complete exemplar evaluation of cycle efficiency with estimator tool and publicize results

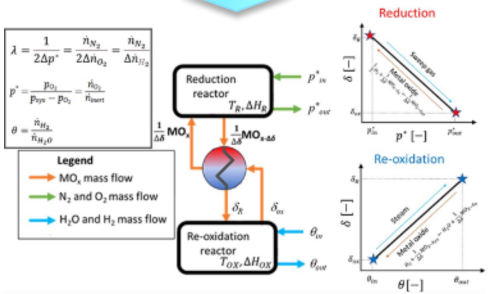
Thermodynamic parameters (from thermo-gravimetric analysis)



Hydrogen production and kinetic parameter (from flow reactor)







Cycle efficiency estimation

Some Exemplar Materials:
BCM: $BaCe_{0.25}Mn_{0.75}O_3$
HEPO: $La_{1/6}Pr_{1/6}Nd_{1/6}Gd_{1/6}Ba_{1/6}Sr_{1/6})MnO_3$
LSM20: $La_{0.8}Sr_{0.2}MnO_3$

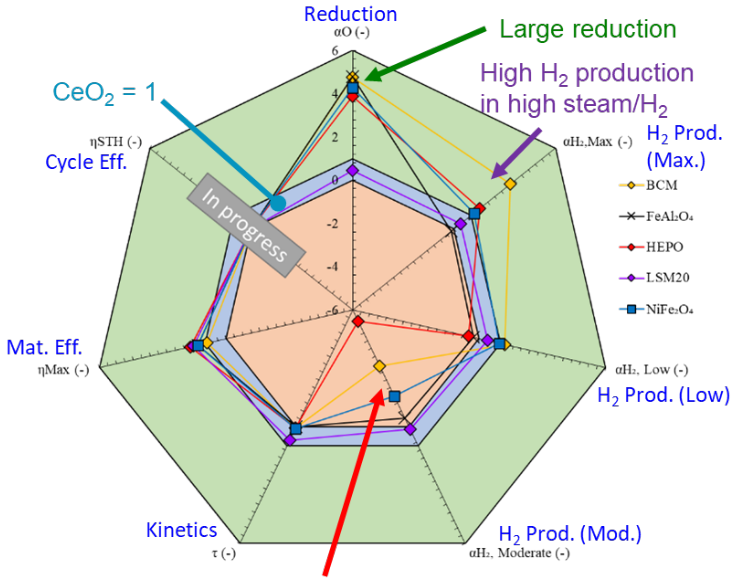
Exemplar Material Commercial Viability Study

STCH Lab R&D Accomplishments

Metrics	Descriptor	Target Values
Cycle Efficiency (STH)	Solar-to-hydrogen conversion efficiency derived from detailed cycle analysis using a thermodynamic model based on specific plant operational assumptions	$\eta_{STH} > 26\%$
Material Efficiency	$\frac{\Delta G^o_{WS}}{\Delta H^o_O}$ is the maximum possible thermal efficiency of the two-step process. (ΔG^o_{WS} evaluated at 25 °C)	$\eta_{Max} > 50\%$
Reduction Capacity	mmol O / mol atom in solid reduced @ neutral low condition	$\alpha_O > 5$
STCH Capacity (Maximum Yield)	mmol H_2 / mol atom in solid reduced @ neutral low condition, oxidized in pure H_2O @ optimal T_{OX} for material	$\alpha_{H2,Max} > 5$
STCH Capacity (Low Yield)	mmol H_2 / mol atom in solid reduced @ neutral low condition, oxidized in steam-to-fuel ratio H_2O/H_2 = 1000 @ optimal T_{OX} for material	$\alpha_{H2,Low} > 2.5$
STCH Capacity (Moderate Yield)	mmol H_2 / mol atom in solid reduced @ neutral low condition, oxidized in steam-to-fuel ratio H_2O/H_2 = 100 @ optimal T_{OX} for material	$\alpha_{H2,Mod} > 1$
Kinetic Performance	Time to 90% of $\alpha_{H2,Max}$ in pure H_2O at optimal T_{OX} for specific material in a dispersed powder configuration	$\tau > 0.20$

Key accomplishment:

- ***Evaluation framework created and metrics identified***
- ***Weakness of exemplars in low steam/H_2 ratio → critical need for new materials***

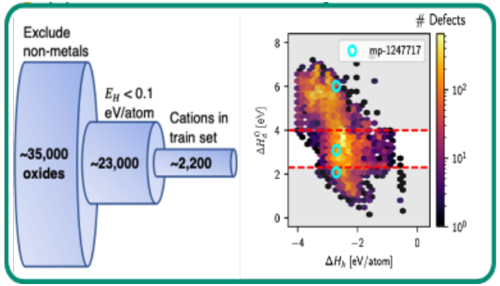


Exemplars normalized to state-of-the-art CeO_2

High Throughput Screening of Materials Project: Version 2
STCH Lab R&D Accomplishments

ML screens 10,000’s of MP structures in minutes that would take 1,000’s of DFT months

Metric	Requirement
Frac. of defects w/ $\Delta H_d^0 > 2.3$ eV	$x_{\min} = 1$
Frac. of defects w/ $\Delta H_d^0 \in [2.3, 4.0]$ eV	$x_{\mathrm{rng}} > 0$
STCH operating range conditions (P_{O_2})	$\Delta\mu'_{O_2}$
Compound stability range	$\Delta\mu_{O_2}^{\phi_H < \{0,\, 0.1, \ldots\}}$
Stable in the target range	$\Delta\mu_{O_2}^{\phi_H < X} \cap \Delta\mu'_{O_2}$

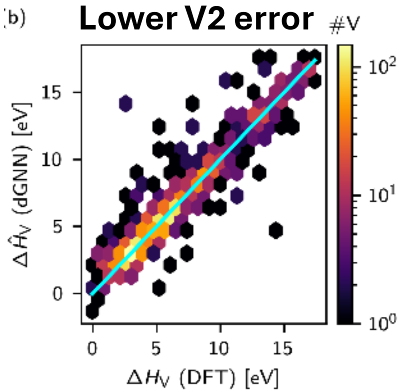


- **V2 training data** = V1 + V1 validation + lit. + new cations

Data Source	#Hosts	#V$_O$	#V$_M$
V1	199	795	686
{Ga,Cr,Pr,Sn}-containing	23	75	57
(SrLa)(AlCoFeMn)O_3 alloys	12	12	0
SCM	2	86	0
BXM	4	18	9
Quat.+ Perovskites	4	8	13
ABO_3	29	43	0
V2 Totals	273	1037	765

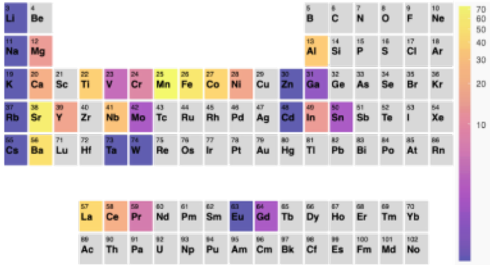
Key accomplishments:

- Version 2 (V2): More compounds for training and more elements included
- Improved ΔH_V MAE for unseen compounds from ~0.5 eV to ~0.4 eV.
- New approach → target “unexpected” STCH compounds for experimental validation



- New cations in V2: V, Pr, Sn, Cr, Ga, Gd, Cs, Rb, Eu, Li, Na, K, Zn, Cd, Mo, W, and Ta

- Prevalence of training compounds containing a given cation

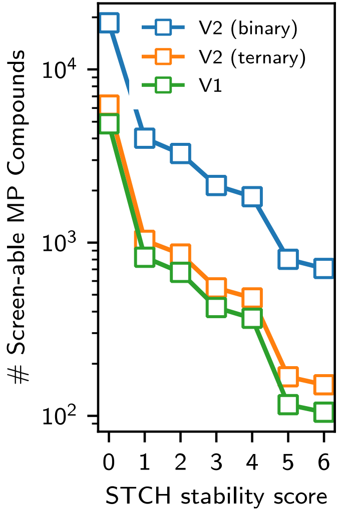


MAE = mean absolute error
MP = Materials Project (https://materialsproject.org/)

High Throughput Screening of Materials Project: Version 2

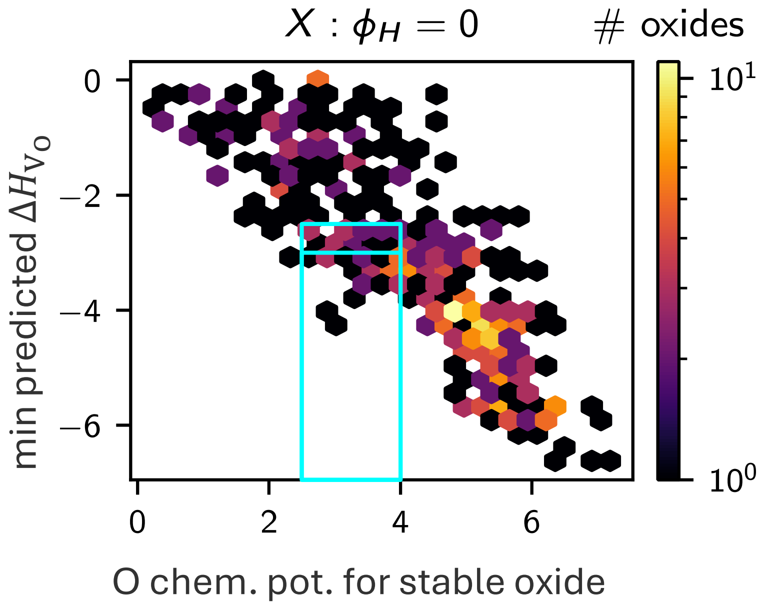
STCH Lab R&D Accomplishments

V2: 10x increase in high stability oxides with desired thermo.



- **~30x reduction** in # of oxides with STCH Stability Score = 6 vs. 0
- BUT… V2 screening will **~10x increase** # of oxides from V1 screening with STCH Stability Score = 6

Identify candidates for experiment in STCH "Golidilocks zone"



Computationally validate with high-throughput DFT

- Between ~50-400 new oxides targeted for DFT calc. of ΔH_{V_O}

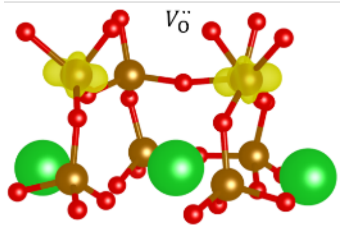
10x more predicted oxides → next step of model validation with computation and experiment

High Throughput Screening of MP Identified New STCH Materials

STCH Lab R&D Accomplishments

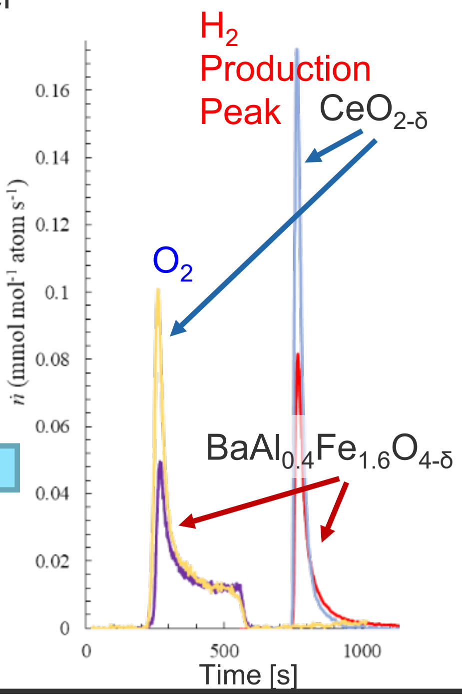
Predicted V1 STCH Compounds → Water-splitters!

$BaFe_2O_4$ – predicted water splitter
(*Al → increased hi-T stability*)



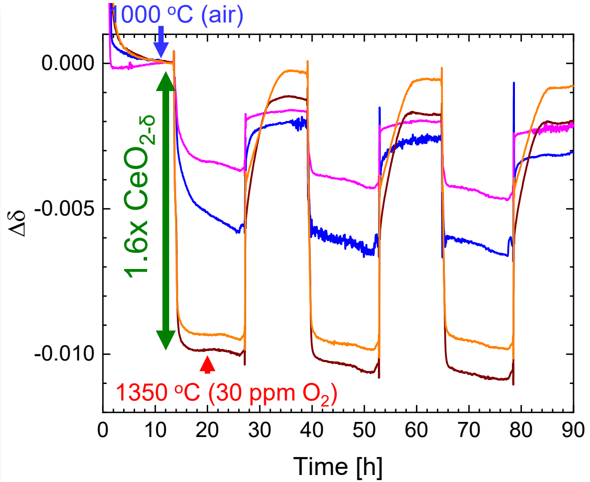
DFT → oxygen vacancy preferred vs. cation defects

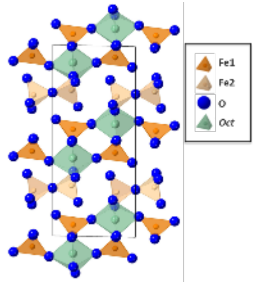
Fe-rich particles formed *in situ* TEM



Identified fabrication and stability challenges in other predicted V1 compounds

$(Ba,Sr)_6Oct_2Fe_4O_{15}$ family → Δδ > CeO_2





STCH screening protocol[1] → $Ba_6Y_2Fe_4O_{15}$ is best
(flow reactor testing next)

[1]*Sanders et al., Front. Energy Res. 10:856943 (2022)*

Milestone accomplishment: >10 new compositions identified from V2 for STCH validation

- Selected by "ease" of fabrication, melting point, ΔH_V, and stability
- Examining unexpected STCH compounds

STCH Summary and Proposed Future Work

Summary:

- Evaluated exemplar materials' potential to meet DOE STCH technology performance targets using a technology assessment methodology developed in this project. Exemplars have attractive H_2 production in dilute H_2/steam, but in concentrated conditions, only one is competitive with state-of-the-art ceria.
  → Need for new materials
- Successfully demonstrated a water splitting material predicted from theory-guided design of materials using a Machine Learning algorithm developed in this project.

Proposed Future Work:

- STCH Lab R&D
  - Apply technology assessment methodology derived in this project to evaluate viability of the >10 predicted V2 STCH materials to meet DOE STCH technology performance targets.
  - Complete technology assessment framework by evaluating exemplars using cycle efficiency model and publicize
  - Continue validation and development of machine learning model for theory-guided design of materials
- Leverage HydroGEN nodes to enable successful completion of new seedling projects.

Any proposed future work is subject to change based on funding levels

Cross-Cutting Modeling Accomplishments: Tadashi Ogitsu

Participating Labs: LLNL, LBNL, NREL, SNL, INL

Presented by: Anh Tuan Pham

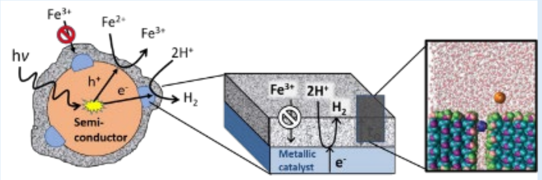
Project ID # P148E

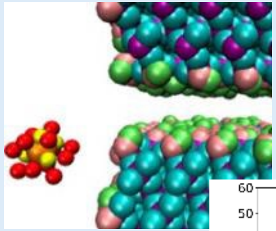
Priorities for cross-cutting modeling activities

Design	• Provide **design guidance** for optimizing materials, components, and devices
Search	• Enable machine learning/data science approaches for **rapid materials discovery**
Explain	• **Deconvolute** key factors that are hard to be accessible through direct experiments
Prioritize	• **Prioritize investments** by assessing the most important factors under operating conditions

Accomplishments of low-temperature technologies (PEC/LTE)
Atomistic insights into transport, OER activities, stability

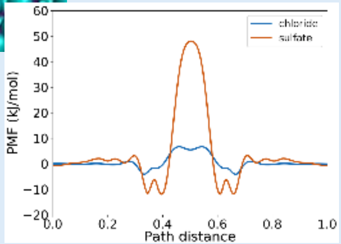
PEC: Protective layers





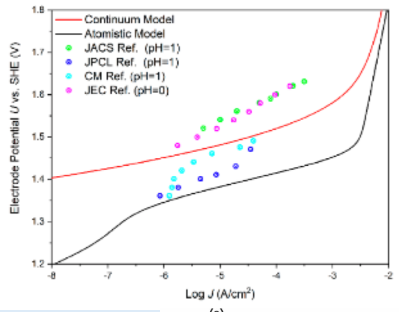
Oxide overlayer for selective transport

Aydin et al., EES Catalyst (Submitted)



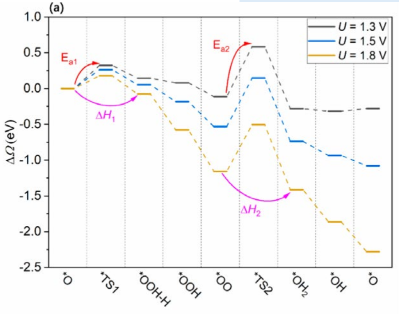
Developed **design principles** for optimizing protective layers

PEC: OER Activity



Developed models for predicting reaction kinetics

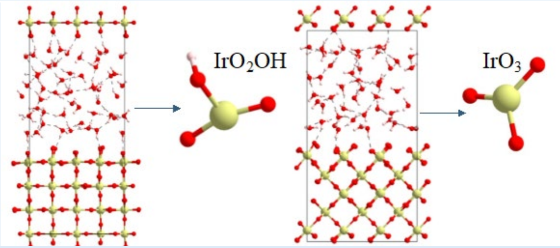
Reaction kinetics as a function of applied potentials



Deconvoluted impacts of operating conditions on activity

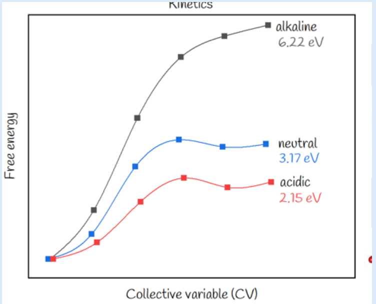
Zhou et al., ACS Appl. Energy. Mater (2023)

LTE: Catalyst Stability



Deconvolute impacts of **surface morphology**

Predict how **pH** influences dissolution kinetics



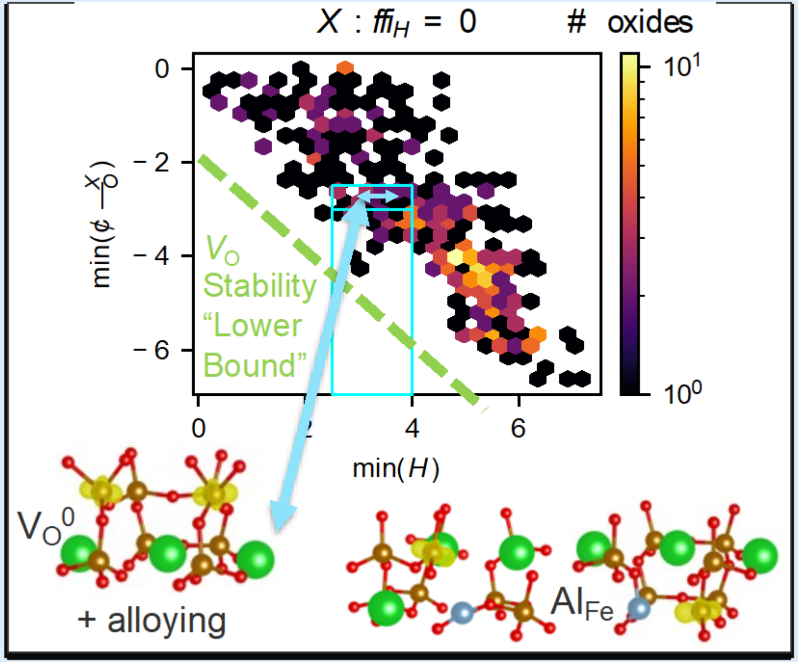
Identified **most important factors** controlling catalyst durability

Zagalskaya et al., (in preparation)

Accomplishments of high-temperature technologies (STCH/HTE)

Understand stability/role of defects at operation condition

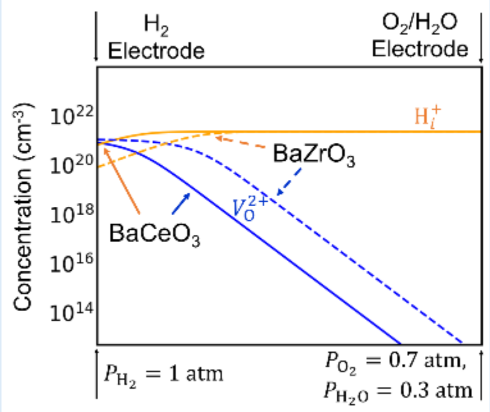
STCH: Expand dataset for oxide discovery



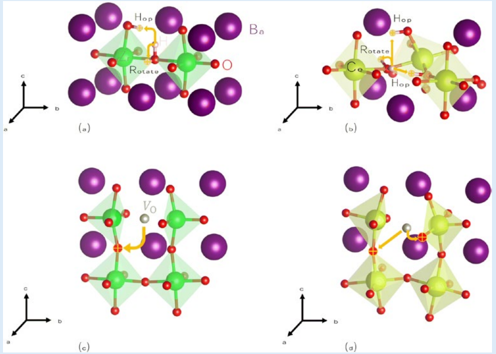
Expand and refine dataset for improving fidelity of ML models for materials discovery

LLNL-SNL. Nat. Comput. Sci. 3, 675 (2023)

HTE: Predict factors controlling transport



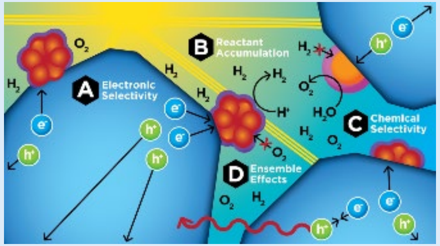
Developed guidance for optimizing **operating conditions** for enhanced ionic conductivity



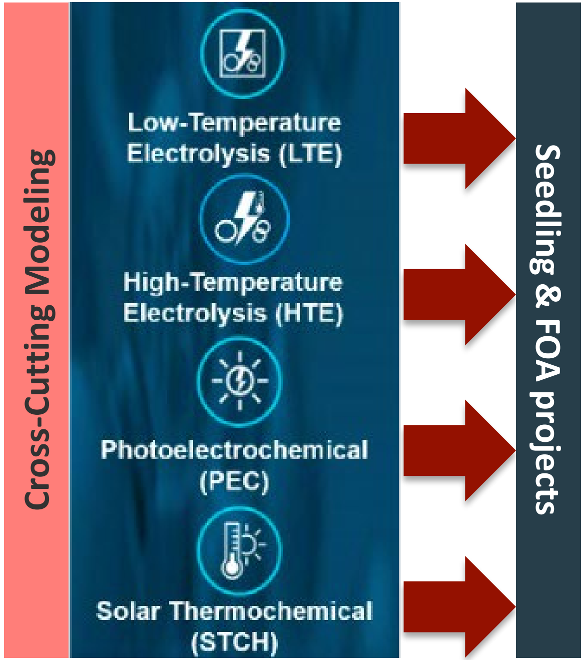
Predicted impacts of **alloying** on ionic conduction

LLNL-INL. Mater. Adv. 4, 6233 (2023)

Collaboration across DOE Hydrogen Program

Centers	Activities
 EFRC: Ensembles of Photosynthetic Nanoreactors (EPN)	• Successfully turned a **seedling project** into a multi-million/institution EFRC project • Continue to engage with EFRCs to create **cross-pollination opportunities** between EERE and BES
EERC: Ionomer-based Water Electrolysis	• Identified common interest, share data and modeling capabilities with CIWE • Developed joint project on development of multiscale simulations for **predicting ionomer degradation**
EPSCoR: Fe based non-PGM OER catalyst	• Support training and **STEM education and workforce development** for hydrogen economy • LLNL team committed to **diversity and inclusion**, and career development (6 early careers with 3 female PDs)

Summary & Proposed Future Work



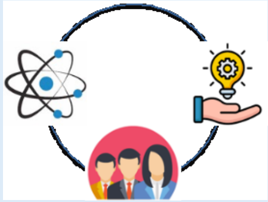
5 publications & 8 invited presentations

Enhance modeling capabilities to achieve HFTO targets

- Develop capabilities to access impacts of materials corrosion on long-term performance
- Develop capabilities to predict how materials & usage variability influence performance and lifetime
- Address the "small data" problem to enable AI/ML approaches for materials discovery and optimization

Foster collaboration & engagement

- Foster collaboration with other offices (DOE-BES, ARPA-E)



- Train next-generation workforce in multiscale simulation through partnerships with leading academic institutions
- Enable and strengthen international partnerships

Any proposed future work is subject to change based on funding levels

General Consortium Proposed Future Work

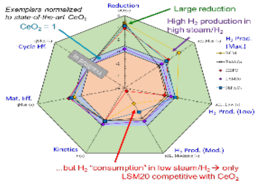
- Develop a DEIA/Community benefits plan
- Lead the AWSM community: develop and socialize technology performance and durability metrics required to meet DOE cost targets, along with benchmarking against these metrics and show year-to-year progress
- Develop STCH and PEC reactors for on-sun testing and capability for on-sun testing
- Perform long-term durability tests to understand the degradation mechanisms and improve the AWS technologies
- Continue collaborative and integrated research on the five HydroGEN lab R&D projects
  - Achieve the HydroGEN Lab R&D FY24 Annual milestones
- Core labs will execute HydroGEN lab nodes to enable successful new Lab- and FOA-awarded project activities
  - Core labs' interaction with a specific project will end if that project does not achieve its go/no-go decision metric
- Continue to actively engage with the Water Splitting Technologies Benchmarking and Protocols project team and participate in workshop, develop protocols & technology roadmaps, and validate protocols.
- 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, LTE, HTE, PEC, and STCH communities
- Continue to develop a user-friendly, information rich, and relevant HydroGEN website and migrate it to a new content management system platform
- Conduct outreach via conference organizations, presentations and participation, benchmarking workshops, website updates and news, publications, and generally socializing the HydroGEN EMN concept to the community

Any proposed future work is subject to change based on funding levels

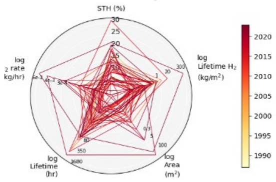
Summary – HydroGEN Consortium:
Advanced Water-Splitting Materials (AWSM)

HydroGEN fosters cross-cutting innovation using theory-guided applied materials R&D to accelerate the time-to-market and advance all emerging water-splitting pathways to enable clean, low cost, and sustainable low-cost hydrogen production

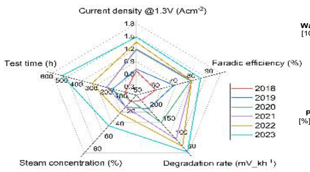
STCH



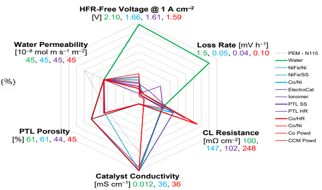
PEC



p-SOEC



AEMWE



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- **Accelerating** the **early-stage AWS technologies** by using the consortium approach to address the critical R&D gaps of each AWS technology with the goal of improving the performance and durability and lower the cost of hydrogen production
- **Achieving technical progress** towards achieving HydroGEN EMN annual milestones
  - 5 HydroGEN lab R&D projects (AEME, p-SOEC, MS-SOEC, PEC, STCH, modeling)
  - Developing figure of merits and metrics to show progress and focus on impactful R&D to enable Hydrogen Shot cost target
  - Collaborating with 11 new solar fuel and 13 new electrolysis projects
- Continuing to connect with H2NEW consortium via **cross-cutting modeling and materials development**
- Continuing to **develop technology roadmaps and standard protocols** for each AWS technology, publishing protocols, engaging with and disseminating information to the community, and validating protocols
- Continuing **to develop Data Hub repository, tools, and metadata**; upgrading application infrastructure to maintain security and cyber standards. (https://datahub.h2awsm.org/)
- Continuing to **connect users to capabilities, publications, research highlights**, contacts, and the Data Hub via the HydroGEN website (www.energy.gov/eere/h2awsm)
- Continuing to develop a diverse STEM workforce, leadership, and community

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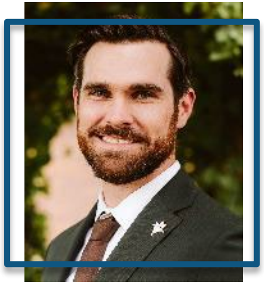

James Vickers

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NREL Team

Huyen Dinh, Lead
Principal Investigators:

Shaun Alia
Bryan Pivovar
Sara Havig
Natasha Headland Nguyen
Rachel Hurst
Emily Harrell
Christina Vader
Eric Payne
Angel Medina-Drago
Megan Grimes
Robert Bell
Guido Bender
Todd Deutsch
Michael Dzara
David Ginley
Steve Harvey
Katie Hurst
Jamie Kee
Stephan Lany
Ross Larsen
Alon Lidor
Mai-Anh Ma
Zhiwen Ma
Janna Martinek
Scott Mauger
Chris Muzzillo
Judy Netter
Genevieve Saur
Sarah Shulda
Myles Steiner
James Young
Andriy Zakutayev
Kai Zhu

LBNL Team

Joel Ager, Lead
Principal Investigators:

Peter Agbo
Oliva Alley
Hanna Breunig
Ethan Crumlin
Walter Drisdell
Dan Gunter
Jinghua Guo
Frances Houle
David Larson
Ahmet Kusoglu
Xiong Peng
David Prendergast
Francesca Toma
Michael Tucker
Adam Weber

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SNL Team

Anthony McDaniel, Lead
Principal Investigators:

Andrea Ambrosini
Kenneth Armijo
Sean Bishop
Arielle Clauser
Eric Coker
Bert Debusschere
Tyra Douglas
Cy Fujimoto
Pinwen Guan
Keith King
Mark Rodriguez
Josh Sugar
Matthew Witman

LLNL Team

Tadashi Ogitsu, Lead
Principal Investigators:

Sarah Baker
Monika Biener
Alfredo Correa Tedesco
Thomas Yong-Jin Han
Tae Wook Heo
Jonathan Lee
Christine Orme
Tuan Anh Pham
Christopher Spadaccini
Tony Van Buuren
Joel Varley
Trevor Willey
Brandon Wood
Marcus Worsley
Timofey Frolov

INL Team

Dong Ding, Lead
Principal Investigators:

Micah Casteel
Rebecca Fushimi
Dan Ginosar
Gabriel Ilevbare
Wei Wu
Qian Zhang