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, Francesca Toma, 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:** June 6, 2023

**DOE Hydrogen Program**

**2023 Annual Merit Review and Peer Evaluation Meeting**

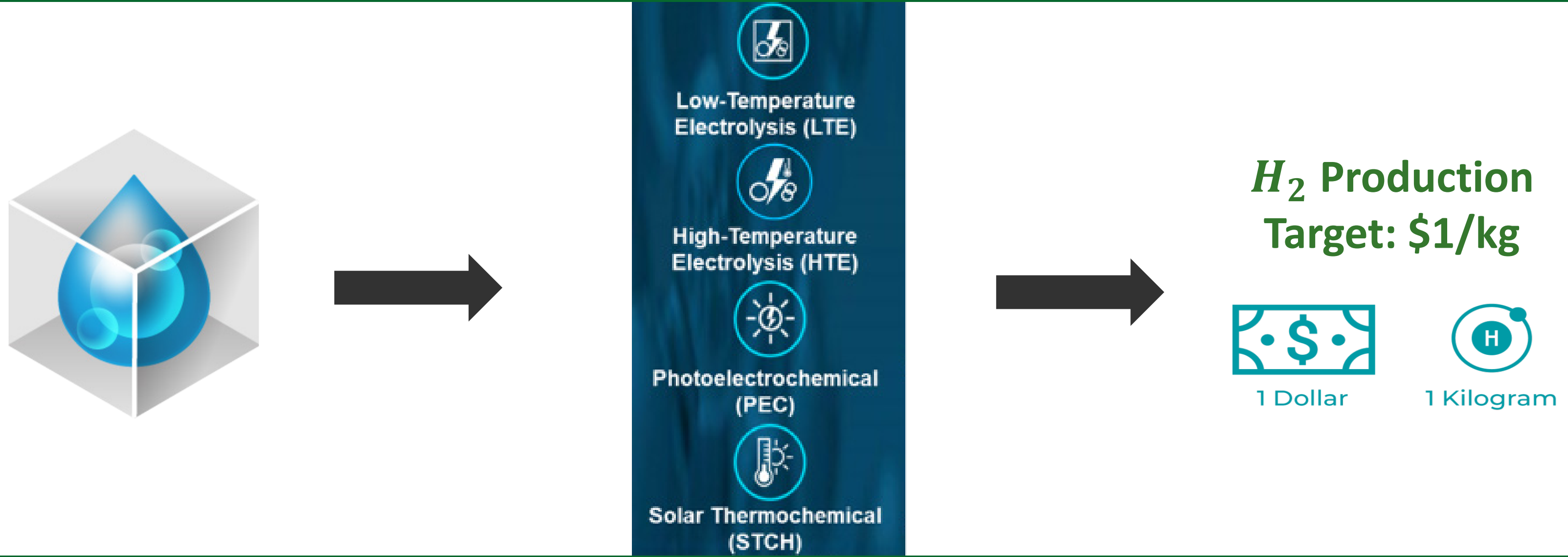
Project ID # P148

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.



Low-Temperature Electrolysis (LTE)

High-Temperature Electrolysis (HTE)

Photoelectrochemical (PEC)

Solar Thermochemical (STCH)

**$H_2$ Production Target: \$1/kg**

1 Dollar

1 Kilogram

***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: $52.275M*

| | |
|---|---|
| **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** | Planned: $10.45M |

## Barriers

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

## Partners

## National Lab Consortium Team

NREL Transforming ENERGY

Lawrence Livermore National Laboratory

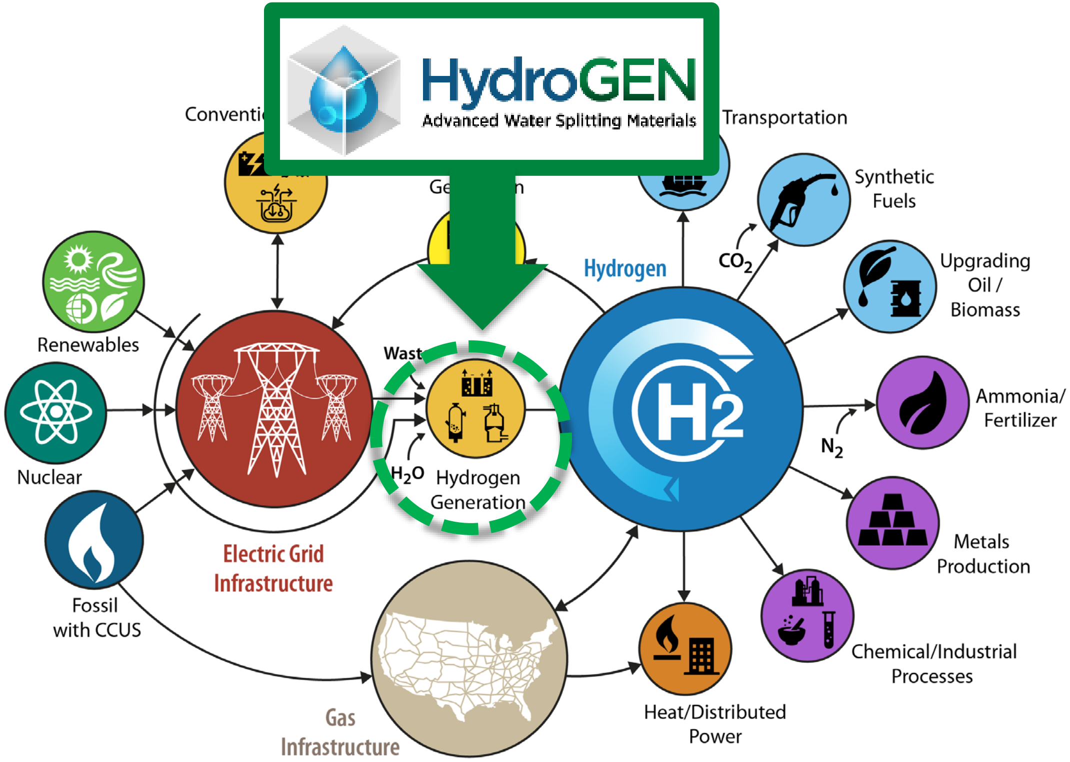
Sandia National Laboratories

INL Idaho National Laboratory

BERKELEY LAB

# H2@Scale: Enabling Affordable, Reliable, Clean and Secure energy

## Relevance and Impact



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

## *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 $H_2$ in the US

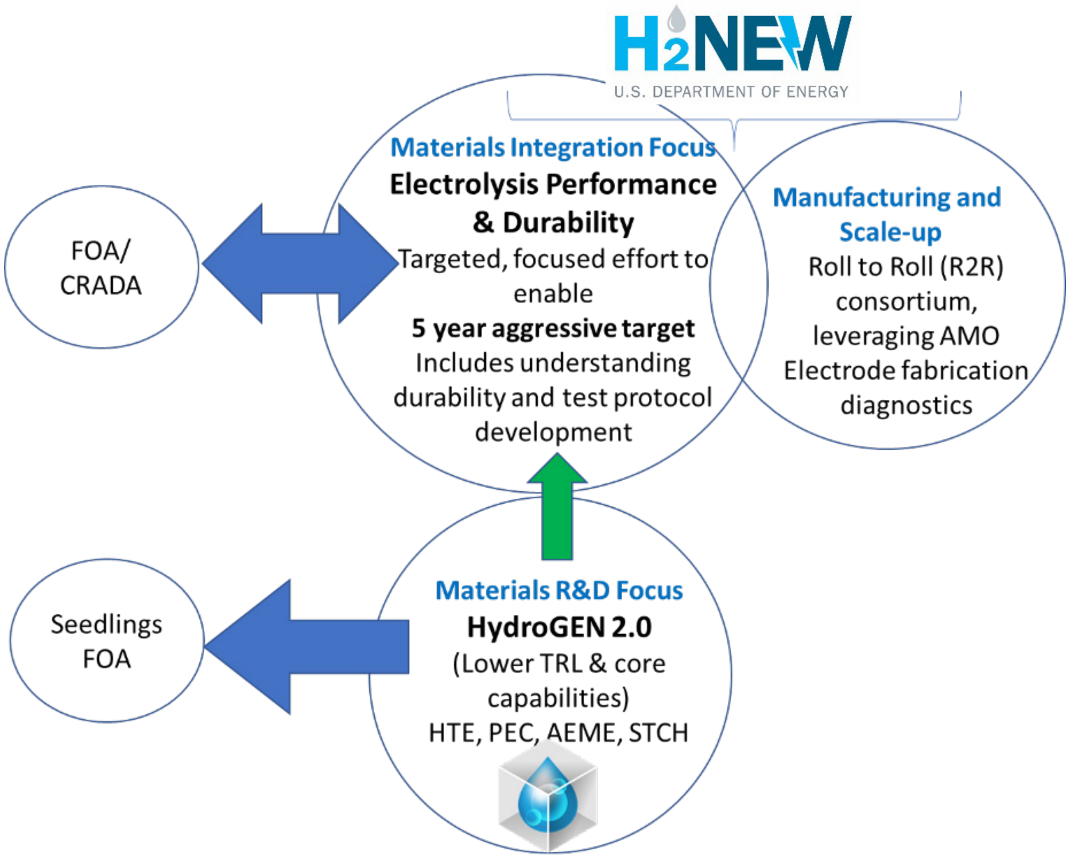
Economic potential: 2x to 4x more

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.

# HydroGEN Materials R&D Feeds to H2NEW Materials Integration

## Approach and Relevance



H2NEW

U.S. DEPARTMENT OF ENERGY

FOA/ CRADA

**Materials Integration Focus**

**Electrolysis Performance & Durability**

Targeted, focused effort to enable

**5 year aggressive target**

Includes understanding durability and test protocol development

**Manufacturing and Scale-up**

Roll to Roll (R2R) consortium, leveraging AMO

Electrode fabrication diagnostics

Seedlings FOA

**Materials R&D Focus**

**HydroGEN 2.0**

(Lower TRL & core capabilities)

HTE, PEC, AEME, STCH

H2NEW | Hydrogen from Next-generation Electrolyzers of Water

U.S. DEPARTMENT OF ENERGY

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

HydroGEN **2.0 (lower TRL AWS)**

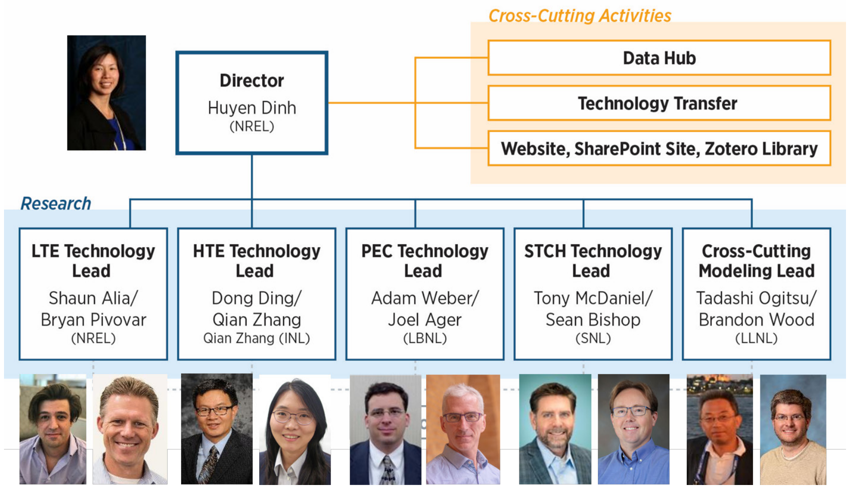
- **Alkaline exchange membrane (AEM) electrolysis**
- **Metal-supported SOEC (MS-SOEC)**
- **Proton-conducting SOEC (p-SOEC)**
- **Photoelectrochemical (PEC)**
- **Solar thermochemical (STCH)**

# HydroGEN Lab R&D + Lab Capability Support

## EMN Collaboration and Approaches

### HydroGEN 2.0: Lab R&D

Early-Stage Materials R&D Projects



*Cross-Cutting Activities*

- Data Hub
- Technology Transfer
- Website, SharePoint Site, Zotero Library

**Director**
Huyen Dinh
(NREL)

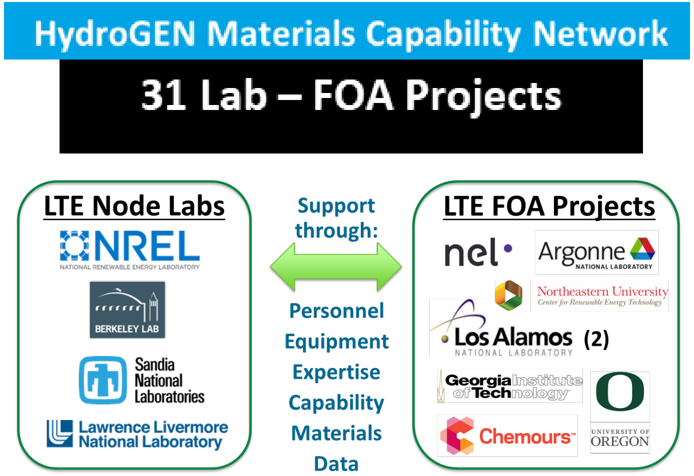
*Research*

| LTE Technology Lead | HTE Technology Lead | PEC Technology Lead | STCH Technology Lead | Cross-Cutting Modeling Lead |
|---|---|---|---|---|
| Shaun Alia/<br>Bryan Pivovar<br>(NREL) | Dong Ding/<br>Qian Zhang<br>Qian Zhang (INL) | Adam Weber/<br>Joel Ager<br>(LBNL) | Tony McDaniel/<br>Sean Bishop<br>(SNL) | Tadashi Ogitsu/<br>Brandon Wood<br>(LLNL) |

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

### HydroGEN 1.0: Lab Support

Lab capabilities + experts support projects



**HydroGEN Materials Capability Network**

**31 Lab – FOA Projects**

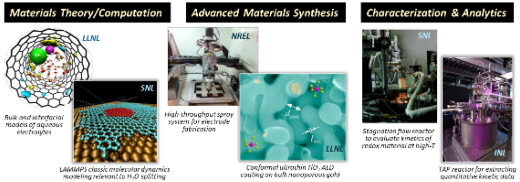
**LTE Node Labs**
NREL National Renewable Energy Laboratory
Berkeley Lab
Sandia National Laboratories
Lawrence Livermore National Laboratory

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

**LTE FOA Projects**
nel
Argonne National Laboratory
Northeastern University Center for Renewable Energy Technology
Los Alamos National Laboratory (2)
Georgia Institute of Technology
Chemours
University of Oregon

# Effectiveness of HydroGEN EMN Framework

## Collaboration / Accomplishments, Streamline Access



*Materials Theory/Computation*

*Advanced Materials Synthesis*

*Characterization & Analytics*

*Bulk and interfacial models of aqueous electrolytes*

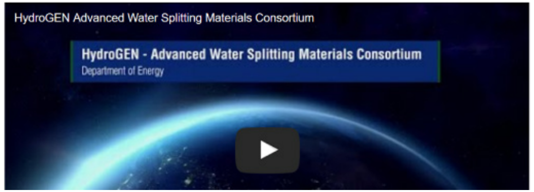
*LAMMPS classic molecular dynamics modeling relevant to $H_2O$ splitting*

*High-throughput spray system for electrode fabrication*

*Conformal ultrathin $TiO_2$ ALD coating on bulk nanoporous gold*

*Stagnation flow reactor to evaluate kinetics of redox material at high-T*

*TAP reactor for extracting quantitative kinetic data*



HydroGEN Advanced Water Splitting Materials Consortium

**HydroGEN - Advanced Water Splitting Materials Consortium**

Department of Energy

**Non-Disclosure Agreement (NDA)**
- Information Disclosure

**Intellectual Property Management Plan (IPMP)**
- IP Protection

**Materials Transfer Agreement (MTA)**
- Freedom to Operate

**Cooperative Research and Development Agreement (CRADA)**
- Collaboration

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

**222 Publications, Impact factor* = 2.68**
**5,653 citations, 436 authors**

**4 community benchmarking workshops**

**33 project NDAs, 2 MTAs**

**46 capabilities utilized across 6 labs**

**STEM Work Force Development**

**Diverse leadership and community**

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

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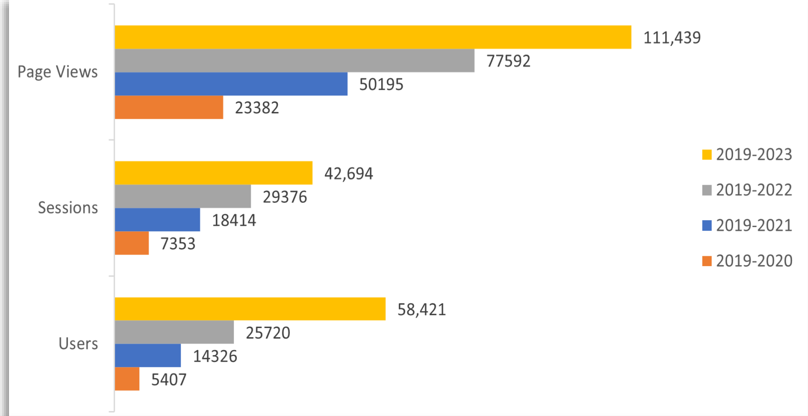
*Field-weighted citation impact (FWCI) indicates how the number of citations received by the Publication Set's publications compares with the average number of citations received by all other similar publications in Scopus.

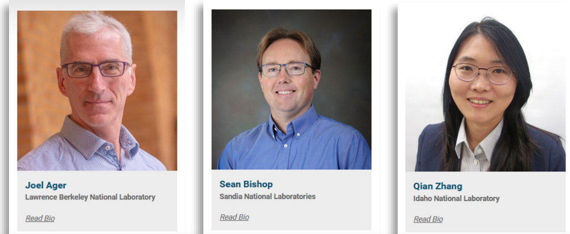
# Effectiveness of HydroGEN Framework: Website Outreach

**https://h2awsm.org**

Website connects users to capabilities, publications, research highlights, contacts, and the Data Hub



Cumulative website usage since inception continues to increase, especially for site users and page views

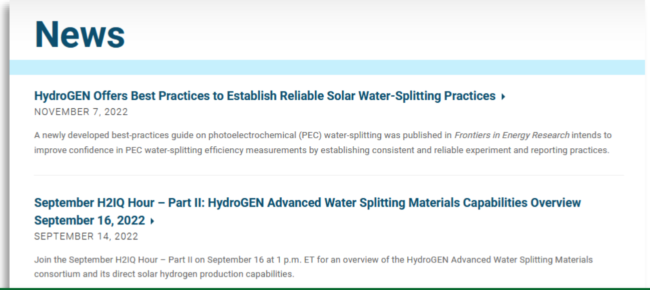


**Joel Ager**
Lawrence Berkeley National Laboratory
*Read Bio*

**Sean Bishop**
Sandia National Laboratories
*Read Bio*

**Qian Zhang**
Idaho National Laboratory
*Read Bio*

New Steering Committee page profiles spotlight three new representatives from our member labs and DOE, serving as consortium capability experts



**News**

**HydroGEN Offers Best Practices to Establish Reliable Solar Water-Splitting Practices ▸**
NOVEMBER 7, 2022

A newly developed best-practices guide on photoelectrochemical (PEC) water-splitting was published in *Frontiers in Energy Research* intends to improve confidence in PEC water-splitting efficiency measurements by establishing consistent and reliable experiment and reporting practices.

**September H2IQ Hour – Part II: HydroGEN Advanced Water Splitting Materials Capabilities Overview September 16, 2022 ▸**
SEPTEMBER 14, 2022

Join the September H2IQ Hour – Part II on September 16 at 1 p.m. ET for an overview of the HydroGEN Advanced Water Splitting Materials consortium and its direct solar hydrogen production capabilities.

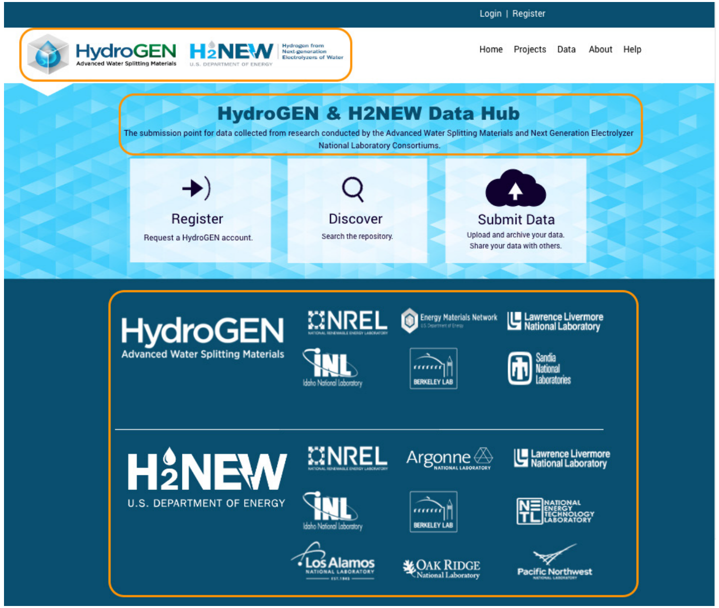
News articles highlight research and accomplishments, including R&D 100 awards honoring two HydroGEN innovations and a PEC best-practices guide

# Collaborative HydroGEN and H2NEW Data Hub

## 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**

## Upcoming development changes to accommodate and represent H2NEW



HydroGEN & H2NEW Data Hub

The submission point for data collected from research conducted by the Advanced Water Splitting Materials and Next Generation Electrolyzer National Laboratory Consortiums.

**Front End**

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

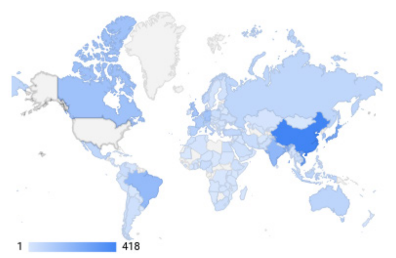
**Data**

- H2NEW Project Creation

# Effectiveness of HydroGEN Framework: Data Hub Accomplishments

*https://datahub.h2awsm.org/*

Visits by Country Outside the United States



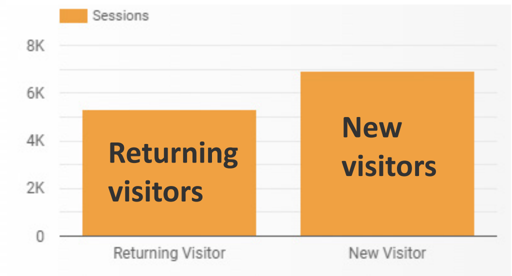
| | Country | Visits ▾ |
|---|---|---|
| 1. | China | 418 |
| 2. | Vietnam | 313 |
| 3. | Japan | 265 |
| 4. | India | 201 |
| 5. | Brazil | 189 |
| 6. | Canada | 159 |
| 7. | Germany | 147 |
| 8. | United Kingdom | 140 |
| 9. | South Korea | 138 |
| 10. | France | 109 |

**Growing & active user community**

| FY18-23 | Site Visitors | Users | Projects | Datasets | Files |
|---|---|---|---|---|---|
| Project to Date | 7,131 | 370 | 61 | 456 | 38,892 |

| | Pageviews | Site Visitors | Sessions | File Downloads |
|---|---|---|---|---|
| FY Totals | 5,954 | 966 | 1,317 | 196 |
| FY18-FY23 | **67,936** | **7,131** | **12,280** | **1,628** |

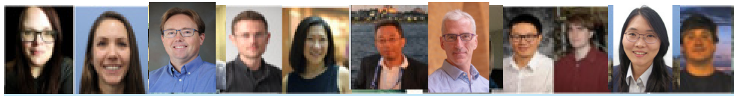
**Session Count by new vs. returning site visitors**



XRD = x-ray diffraction; SFR = stagnation flow reactor; J-V = current vs. voltage data; TEM = transmission electron microscopy

XPS = x-ray photoelectron spectroscopy; TGA = thermal gravimetric analysis; IPCE = incident photon to current efficiency

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



## Data Hub Team 2022-2023 Year in Review

- Ready for upgrade release
- Started development work for future search capabilities
- Created layout for incorporating H2NEW into the HydroGEN Data Hub. Defined H2NEW projects and developed training content.
- Continues to support the authorization and management of user accounts, the user interface, project creation and structure, and dataset upload and publication

### Many Types of Experimental Data

**Material characterization**

•XRD, SFR, XPS, XRF, SEM, TEM, Raman

**Device performance**

•Electrolysis, PEC J-V, IPCE, Tafel plots

**Materials durability data**

•TGA, membrane conductivity

# Community Approach to Benchmarking and Protocol Development for AWS Technologies

## Accomplishments

P170

***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:

- **19 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**
  - **7 LTE, 4 HTE, 5 PEC, 3 STCH**
  - **4,912 total downloads and 36,000 views**
- **4 Annual AWS community-wide benchmarking workshop**
- **Developed high-level roadmaps by AWS technology**

# Science Challenges for HydroGEN 2.0 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***:

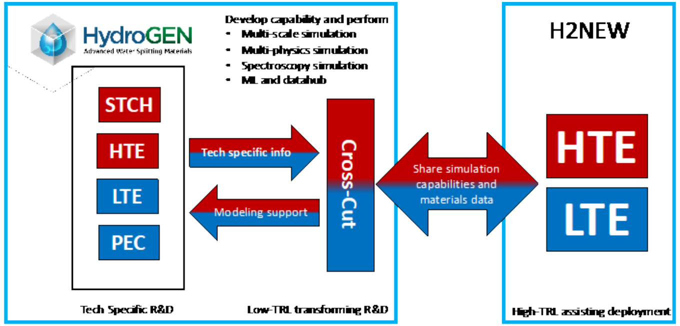
**MS-SOEC**: improve performance and durability with a scale-up cell

**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

The project was not reviewed last year.

The 2021 reviewers' comments were addressed in the 2022 AMR presentation.

# Solar Thermochemical Water Splitting (STCH): Tony McDaniel

## Participating Labs: SNL, NREL, LLNL

Project ID # P148D

# HydroGEN STCH Seedling Projects & Lab Collaboration

Barriers
- Cost
- Efficiency
- Durability

## STCH Node Labs

Sandia National Laboratories

NREL Transforming ENERGY

Lawrence Livermore National Laboratory

**Support through:**

**Personnel**

**Equipment**

**Expertise**

**Capability**

**Materials**

**Data**

## Interactive STCH Projects

ASU Arizona State University

UCSD

Princeton University

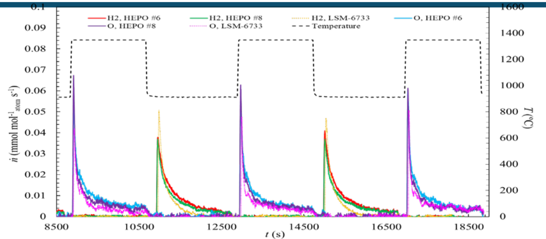
West Virginia University

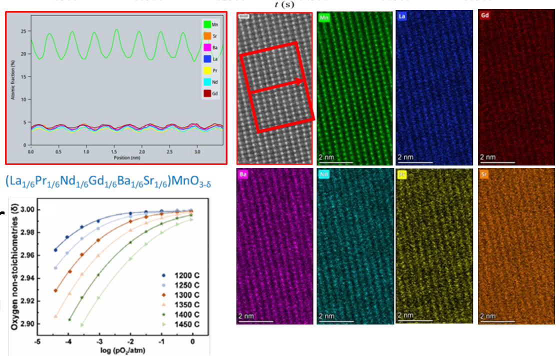
UF University of Florida

# HydroGEN STCH Seedling Projects with Lab Capability Support

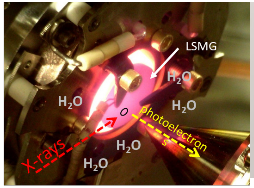
## Technical Accomplishment Highlights

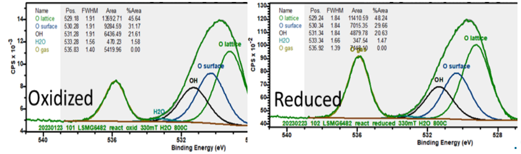
- **(P168, ASU, Princeton and SNL, NREL) Mixed Ionic Electronic Conducting Quaternary Perovskites: Materials by Design for STCH $H_2$:** Theoretical discovered and experimentally validated perovskite $Ca_{2/3}Ce_{1/3}Ti_{1/3}Mn_{2/3}O_3$ with desirable redox thermodynamics for STCH. Material demonstrates greater $H_2$ production capacity than recent promising Sr-La-Mn-Al and Ba-Ce-Mn metal oxide perovskites. This perovskite is unique because A-site $Ce^{4+}$ reduction dominates the redox-activity, instead of the B-site cations seen for all other perovskites.
- **(P194, UCSD, WVU and SNL) High Entropy Perovskite Oxides with Increased Reducibility for STCH:** Discovered and demonstrated a compositionally complex perovskite oxide $(La_{1/6}Pr_{1/6}Nd_{1/6}Gd_{1/6}Ba_{1/6}Sr_{1/6})MnO_3$ that achieves a thermodynamic and kinetic balance for STCH. The combination of a moderate reduction *enthalpy*, a high reduction *entropy*, and preferable surface oxygen exchange kinetics, enables $H_2$ production capacity greater than a $La_{.67}Sr_{.33}MnO_3$ analog and suggests a new class of compositionally complex ceramics for STCH functionality.
- **(P195, UF and SNL, NREL) A New Paradigm for Materials Discovery and Development for Lower Temperature and Isothermal Thermochemical $H_2$ Production:** Developed foamed perovskite structures more suitable for scaled-up operation that have excellent redox stability, and exhibit oxidation kinetics and bulk properties comparable to powder samples. Used eXPS to reveal mechanistic details of water splitting surface chemistry and verify compositional stability in operando.





$(La_{1/6}Pr_{1/6}Nd_{1/6}Gd_{1/6}Ba_{1/6}Sr_{1/6})MnO_{3-\delta}$





# 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).
- Find new materials using the ML model and characterize by detailed calculations, synthesis, and experimental validation.

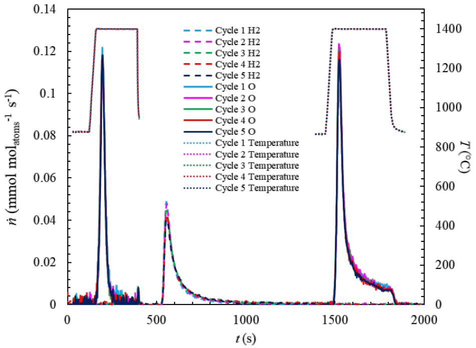
| | |
|---|---|
| **State of the Art (Point A)** | Materials evaluation protocols are absent. Rigorous assessment of the potential for materials to meet DOE STCH technology performance targets is also absent.<br>Materials that efficiently and cost effectively produce $H_2$ remain elusive because increasing both capacity ($\Delta\delta$ at lower $T_{RED}$) and reaction yield in non-stoichiometric oxides has not been demonstrated. |
| **End of Project Milestone (Point B)** | Use the technology assessment methodology derived during the course of this project to evaluate material viability. A selected group of materials will be evaluated for their potential to meet DOE STCH technology performance targets.<br>Demonstrate theory-guided design of materials using ML by establishing the correlations between thermochemical properties and the underlying structure/composition features for a large number (>1000) of compositions and structures. Identify and validate materials that optimize the capacity/yield tradeoff. |

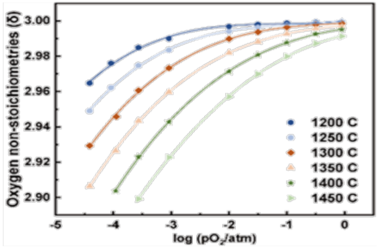
DFT = density functional theory
$T_{RED}$ = reduction temperature

# Exemplar Material Commercial Viability Study

## STCH Lab R&D Accomplishments

- Materials, methods and metrics determined by community consensus (via Benchmarking).
  - Selected performance metrics (*) normalized to $CeO_2$ performance
- Software platform developed for “end to end” processing of experimental data.
  - Will be made available to public
- Collecting data and analyzing performance of exemplar materials.
  - Developed robust TGA and flow reactor experimental protocols





## Performance Conditions and Assumptions:

| Parameter | Neutral |
|---|---|
| Reduction temperature ($T_{red}$) | 1673.15 K |
| Reduction $O_2$ partial pressure ($pO_2$,reduction) | 10 Pa |
| Solid-solid heat recuperation effectiveness ($\varepsilon_{ss}$) | 50% |
| Gas-gas heat recuperation effectiveness ($\varepsilon_{gg}$) | 50% |
| $O_2$ separation efficiency | 10% |
| $H_2/H_2O$ separation efficiency | 10% |

| Metric | Descriptor | Value |
|---|---|---|
| **ideal efficiency** | $\Delta G^o$ (homolysis) / $\Delta H$red (mole O) is the maximum possible thermal efficiency of a two-step process | $\eta_{MAX}$ >50% |
| **cycle thermal efficiency** | Derived from a detailed thermodynamic cycle analysis model using specific assumptions and validated material equation of state; note this is NOT solar-to-$H_2$ conversion efficiency | $\eta_{cyc}$ >34% |
| **kinetic performance** | Time to 90% of $\Delta\delta$ in pure $H_2O$ (≥40 vol%) at near optimal $T_{ox}$ for specific material in a dispersed powder configuration | t >0.20* |
| **$O_2$ capacity** | mmol O / mol atom in solid reduced @ neutral condition | $\alpha_O$ >15* |
| **$H_2$ capacity (max yield)** | mmol $H_2$ / mol atom in solid reduced @ neutral condition, oxidized in pure $H_2O$ (>40 vol%) @ near optimal $T_{ox}$ for material | $\alpha_{H2,MAX}$ >15* |
| **$H_2$ capacity (low yield)** | mmol $H_2$ / mol atom in solid reduced @ neutral condition, oxidized in $H_2O$:$H_2$ ratio of 1000:1 @ near optimal $T_{ox}$ for material | $\alpha_{H2,LOW}$ >15* |
| **$H_2$ capacity (mod. yield)** | mmol $H_2$ / mol atom in solid reduced @ neutral condition, oxidized in $H_2O$:$H_2$ ratio 100:1 @ near optimal $T_{ox}$ for material | $\alpha_{H2,MOD}$ >10* |
| **degradation rate** | Capacity fade similar to batteries, % loss in $\alpha_{H2,MAX}$ over 1000 cycles, may have to extend # of cycles depending on kinetic performance | TBD |
| **material cost** | | TBD |
| **material durability** | Total lifetime $H_2$ produced | TBD |

## Exemplar Materials:

| Material | Class |
|---|---|
| $CeO_2$ | Fluorite, state of the art |
| $La_{0.8}Sr_{0.2}MnO_3$ | “Simple” perovskite |
| $Ba_4CeMn_3O_{12}$ | Complex perovskite, best in class |
| $FeAl_2O_4$ | “Hercynite” spinel, long studied |
| $NiFe_2O_4$ | Spinel |
| $(La_{0.167},Pr_{0.167}Nd_{0.167}Gd_{0.167}Ba_{0.167}Sr_{0.167})MnO_3$ | Polycation perovskite oxide, UCSD formulation |
| Hy2.0 DFT+ML and/or Seedling formulation | ? |

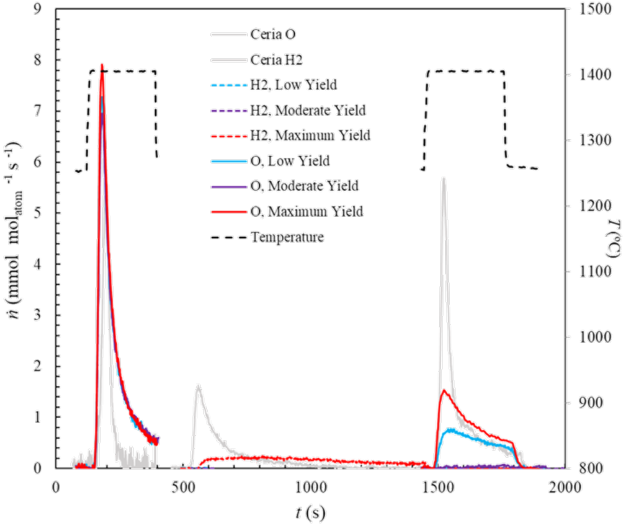
# Results for $CeO_2$ "Baseline" Compound and $FeAl_2O_4$ Exemplar Studies

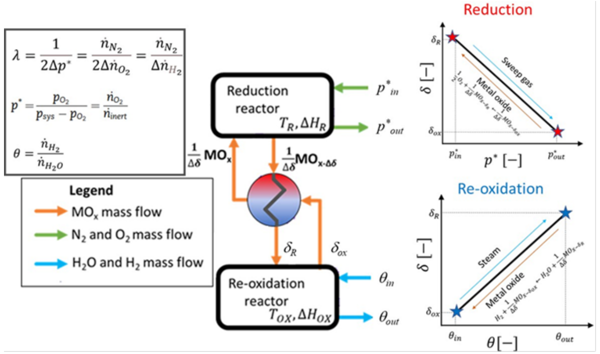
## STCH Lab R&D Accomplishments

| Metric | Value | $CeO_2$ (baseline) | $FeAl_2O_4$* |
|---|---|---|---|
| ideal efficiency | $\eta_{MAX}$ >50% | 54% | 95% |
| cycle thermal efficiency | $\eta_{cyc}$ >34% | 6.45% | ? |
| kinetic performance | t >0.20* | ~150 s | <<0.1 |
| $O_2$ capacity | $\alpha_O$ >15* | 3.4 mmol/mol atom | 2.4-8 |
| $H_2$ capacity (max yield) | $\alpha_{H2,MAX}$ >15* | 3.4 mmol/mol atom | 0.72-? |
| $H_2$ capacity (low yield) | $\alpha_{H2,LOW}$ >15* | 3.4 mmol/mol atom | 0 |
| $H_2$ capacity (mod. yield) | $\alpha_{H2,MOD}$ >10* | 3.4 mmol/mol atom | 0 |
| degradation rate | TBD | stable to cycling | ? |
| material cost | TBD | \$2-6k/mt | \$1-2k/mt<br>based on<br>$MgAl_2O_4$ |
| material durability | TBD | ? | ? |

grey - $CeO_2$, $T_{ox}$=850C

colored - $FeAl_2O_4$, $T_{ox}$=1200C





$$\lambda = \frac{1}{2\Delta p^*} = \frac{\dot{n}_{N_2}}{2\Delta \dot{n}_{O_2}} = \frac{\dot{n}_{N_2}}{\Delta \dot{n}_{H_2}}$$

$$p^* = \frac{p_{O_2}}{p_{sys} - p_{O_2}} = \frac{\dot{n}_{O_2}}{\dot{n}_{inert}}$$

$$\theta = \frac{\dot{n}_{H_2}}{\dot{n}_{H_2O}}$$

| Parameter | Neutral | Model |
|---|---|---|
| Reduction temperature ($T_{red}$) | 1673.15 K | $T_{r,max}$ = 1673.15 K |
| Reduction $O_2$ partial pressure ($pO_2$,reduction) | 10 Pa | $p_{O2, in}$ = 10 Pa |
| Solid-solid heat recuperation effectiveness ($\varepsilon_{ss}$) | 50% | $\eta_{ss}$ = 0.5 |
| Gas-gas heat recuperation effectiveness ($\varepsilon_{gg}$) | 50% | $\eta_{gg}$ = 0.5 |
| $O_2$ separation efficiency | 10% | $\eta_{sep}$ = 0.1 |
| $H_2/H_2O$ separation efficiency | 10% | $\eta_{sep}$ = 0.1 |
| Output $H_2/H_2O$ mole ratio | | $\theta_{out}$ = 0.1 |
| Material oxidation extent ($\delta_{ox}$) | | $\delta_{ox}$ = 0.001 |

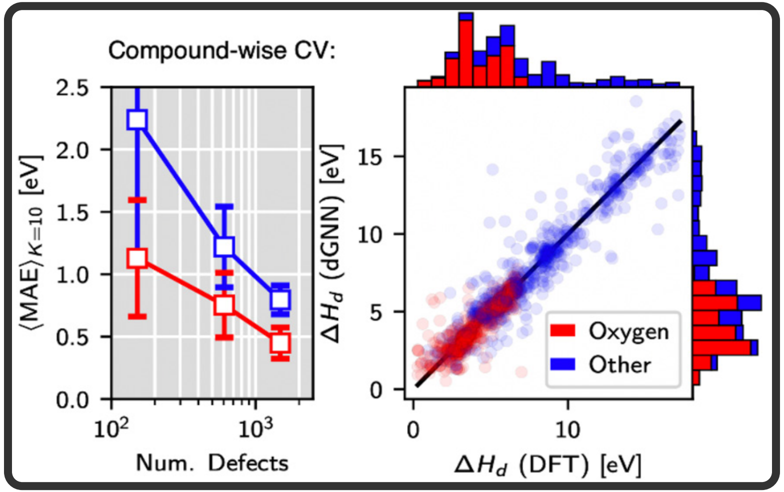
Methodology exposes $FeAl_2O_4$ strengths and weaknesses compared to SOA $CeO_2$.

- Higher ideal efficiency, larger $O_2$ redox capacity, lower material cost (strength)
- Low $H_2$ capacity, slow redox kinetics, extremely low $H_2$ capacity at LOW and MOD yield (weakness)

SOA = state of the art

# High Throughput Screening of Materials Project Using DFT-ML on Round-1 Cations

## STCH Lab R&D Accomplishments



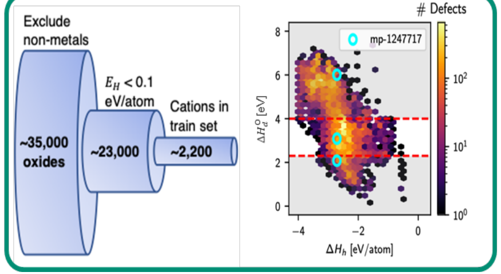
- Expected $\Delta H_{0,d}$ MAE for unseen compounds < 450 meV (threshold for ML to be predictive).
- Model rediscovers known water-splitting oxides and identifies new ones.

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

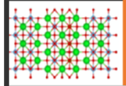
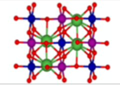
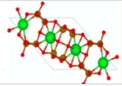
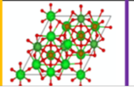
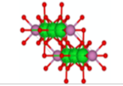
**(1) Co-design of defects and stability for water-splitting**

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

**(2) Screen the Materials Project for all defects**



**(3) Identify targets w/increasingly stringent metrics**

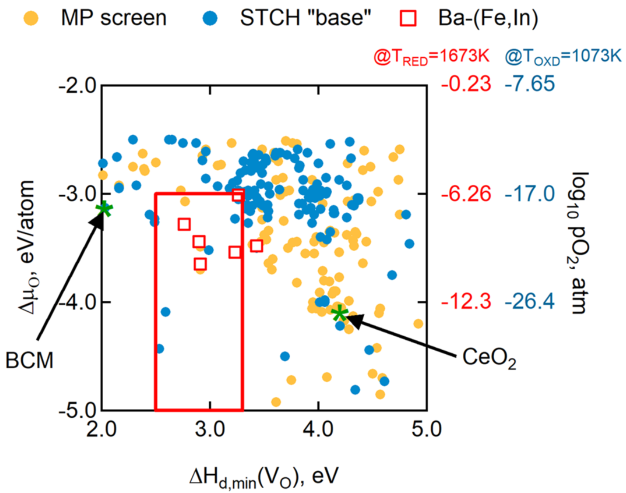
| 197 formulas (48 training) | 114 formulas (33 training) | 34 formulas (17 training) | 16 formulas (11 training) | 9 formulas (9 training) |
|---|---|---|---|---|
| ➢ $x_{\mathrm{min},1} = 1$<br>➢ $x_{\mathrm{rng},1} > 0$<br>➢ $\Delta\mu_{O_2}^{\phi_H < 0.1}$ | ➢ $x_{\mathrm{min},2} = 1$<br>➢ $x_{\mathrm{rng},2} > 0$<br>➢ $\Delta\mu_{O_2}^{\phi_H < 0.1}$ | ➢ $x_{\mathrm{min},3} = 1$<br>➢ $x_{\mathrm{rng},3} > 0$<br>➢ $\Delta\mu_{O_2}^{\phi_H < 0.05}$ | ➢ $x_{\mathrm{min},3} = 1$<br>➢ $x_{\mathrm{rng},3} > 0$<br>➢ $\Delta\mu_{O_2}^{\phi_H = 0}$ | ➢ $x_{\mathrm{min},3} = 1$<br>➢ $x_{\mathrm{rng},3} = 1$<br>➢ $\Delta\mu_{O_2}^{\phi_H = 0}$ |
| $Sr_6Ti_3FeO_{14}$<br>(mp-1645141) | $La_2MnCoO_6$<br>(mp-19208) | $BaSr(FeO_2)_4$<br>(mp-1228024) | $Ba_5SrLa_2Fe_4O_{15}$<br>(mp-698793) | $Ba_3In_2O_6$<br>(mp-20352) |
|  |  |  |  |  |

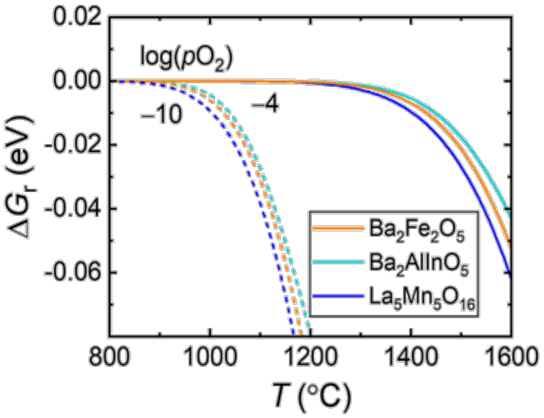
- ➢ Identify all candidates satisfying minimum requirements
- ➢ Identify candidates with increasingly certain performance
- ➢ Mainly IDs known, synthesizable compounds

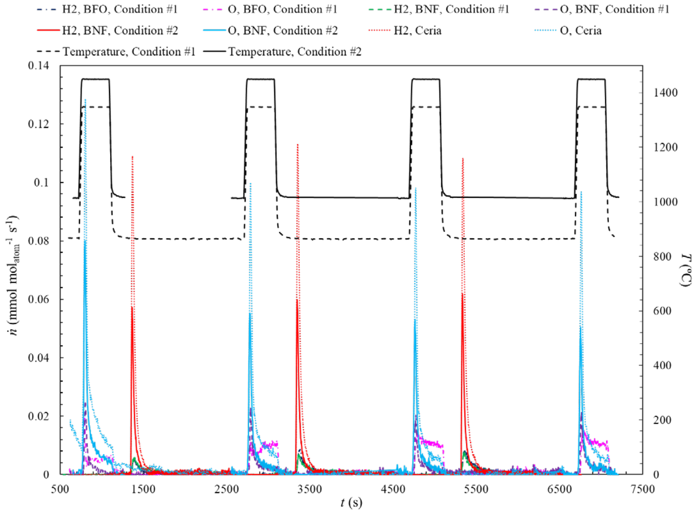
MAE = mean absolute error
MP = Materials Project (https://materialsproject.org/)

# High Throughput Screening of MP Identified New STCH Materials

## STCH Lab R&D Accomplishments



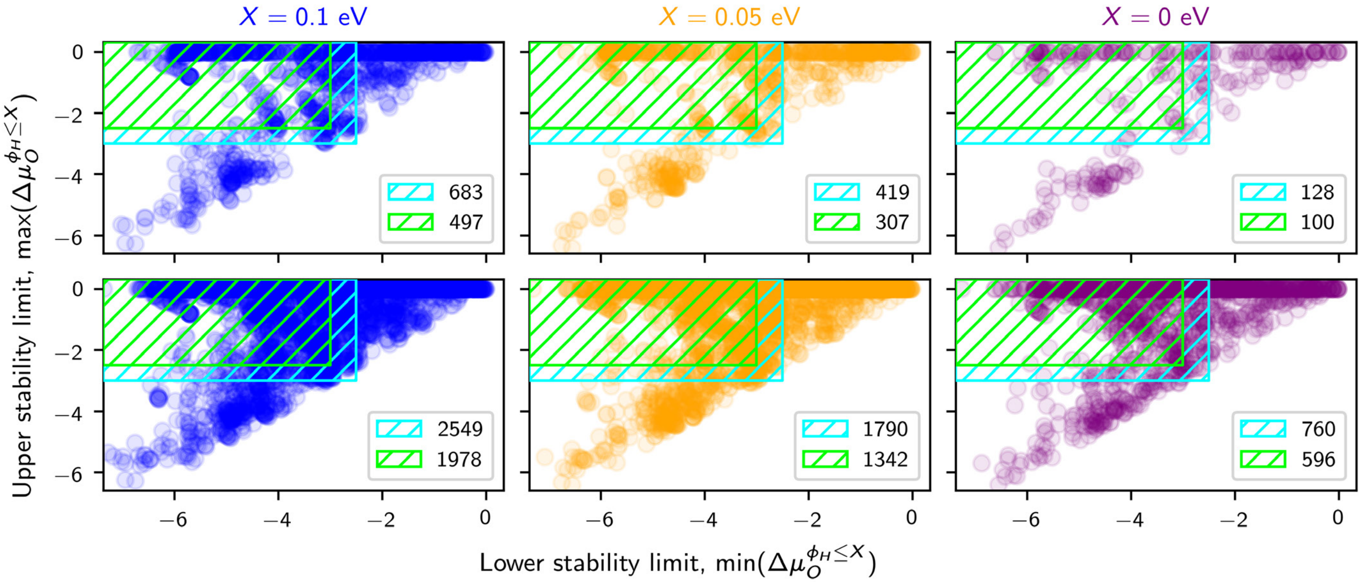




- Created thermodynamic analysis tool that interfaces with the DFT-ML data.
  - Generate T and $pO_2$ dependent free energies from DFT-ML data
  - Bypass time-consuming supercell defect calculations
- Synthesized >10 identified compounds of interest; resulting in ≥ 2 new validated water splitting materials with screening ongoing on others.

# DFT-ML Defect Studies for Training ML on Expanded List of Cations to Reveal More STCH Materials

**STCH Lab R&D Accomplishments**



- Cations used in training DFT-ML model.
  - Round 1 (R1): Al, Ba, Ca, Ce, Co, Fe, In, La, Mg, Mn, Nb, Ni, O, Sr, Ti, Y
  - Round 2 (R2): Cr, Cs, Eu, Ga, Gd, Hf, K, Mo, Na, Nb, Rb, Sn, Ta, V, W, Yb, Zr
- Increase number of screen-able candidates by 4-6x.
  - 100 (R1) compounds, 596 (R1+R2) compounds

# STCH Summary and Proposed Future Work

**Summary:**

- Seedling project successes on discovering new STCH materials enabled by collaboration with HydroGEN by providing experimental and theoretical results using advanced methods.
- Critical evaluation of six exemplar STCH materials on track for completion by end of FY23.
  - Rigorously derived material performance data will inform technology viability assessment
- The ML modeled developed is a potential game changer for high throughput material discovery.

**Proposed Future Work:**

- STCH Lab R&D
  - Use technology assessment methodology derived during this project to evaluate viability of exemplar materials to meet newly formulated DOE STCH technology performance targets
  - Continue theory-guided design of materials using machine learning to identify more redox active materials that optimize the capacity/yield tradeoff
- 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

# High Temperature Electrolysis (HTE) Technical Accomplishments: Dong Ding

## Participating Labs: INL, LBNL, LLNL

Project ID # P148B

# HydroGEN HTE Seedling Projects and Lab Collaboration

**Project-driven tech transfer, resulting in**

- Efficiency
- Yield
- Cost
- Durability
- Manufacturability

## 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

**p-SOEC**

Raytheon Technologies

University of Connecticut

West Virginia University

REDOX Redox Power Systems, LLC

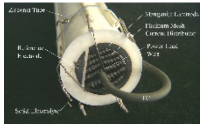
**o-SOEC**

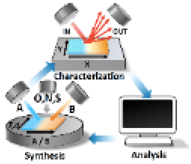
Northwestern University

SAINT-GOBAIN

University of South Carolina

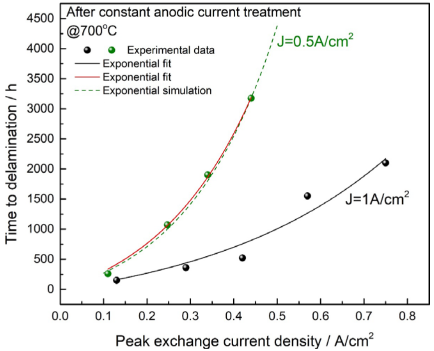
NEXCERIS where energy meets environment

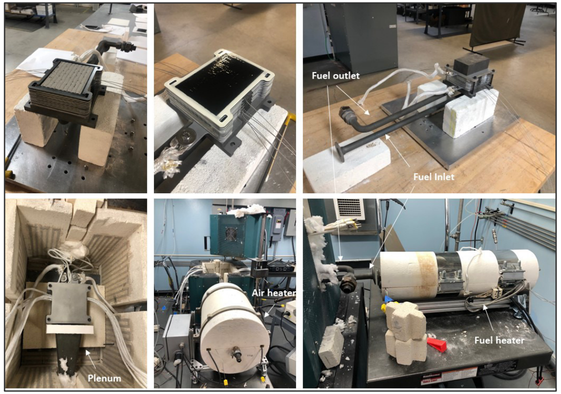


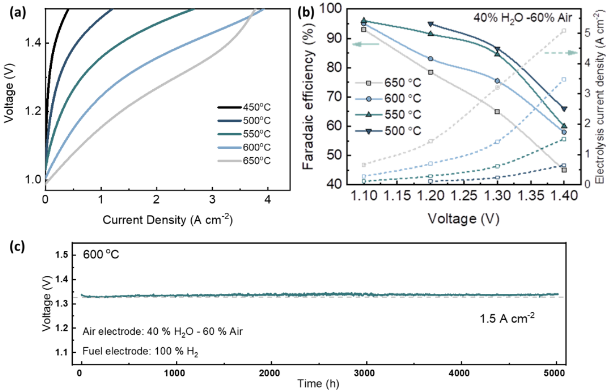


# HydroGEN HTE Seedling Projects with Lab Capability Support
## Technical Accomplishment Highlights

- **(P190, USC, INL and NREL) A Multifunctional Isostructural Bilayer Oxygen Evolution Electrode for Durable Intermediate-Temperature Electrochemical Water Splitting**: Demonstrated a 700$^{o}$C-bilayer oxygen electrode for solid oxide electrolyzers; Established the relationship between exchange current density and time-to-delamination of oxygen electrode for prediction of safe operating current density; Demonstrated high performance of tubular solid oxide electrolyzers.
- **(P188, Nexceris and INL) Advanced Coatings to Enhance the Durability of SOEC Stacks:** Demonstrated large-scale manufacturing at a cost of less than $1/per part (<$3/kW) for a plant that produces 6 million coated interconnects/yr; Explored processing routes and demonstrated capability for scaling of interconnect, monolith and tube coating manufacturing.
- **(P175, WVU and INL) Intermediate Temperature Proton-Conducting Solid Oxide Electrolysis Cells with Improved Performance and Durability**: p-SOEC was developed and demonstrated to operate at a 1.5A/cm$^2$ at 600°C for 5000 h with a degradation rate of ~1mV/kh; Conformal catalyst coating technology was established and proven effective; Defect chemistry model was developed to predict the leakage behaviors of electrolyte under practical conditions.



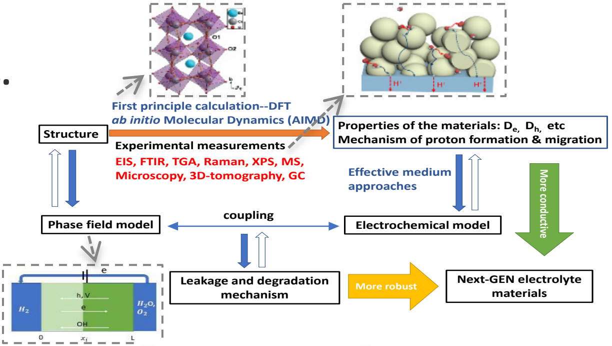




# Combine Multi-Scale Computation and Experiment to Improve Faradaic Efficiency

## HTE Lab R&D p-SOEC Approach

- **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.**



Structure

First principle calculation--DFT

*ab initio* Molecular Dynamics (AIMD)

Experimental measurements

EIS, FTIR, TGA, Raman, XPS, MS, Microscopy, 3D-tomography, GC

Properties of the materials: $D_e$, $D_h$, etc

Mechanism of proton formation & migration

Effective medium approaches

More conductive

Phase field model

coupling

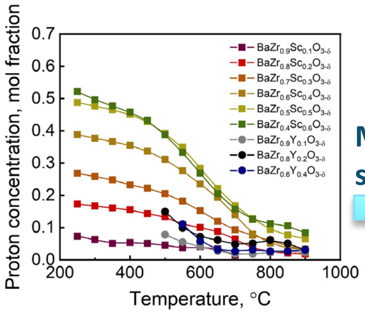
Electrochemical model

Leakage and degradation mechanism

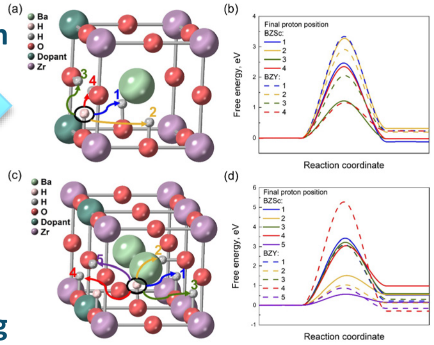
More robust

Next-GEN electrolyte materials

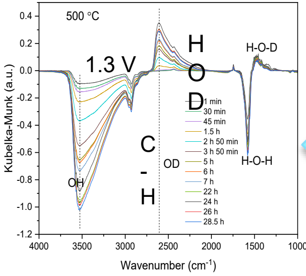
- **Framework:** Established an efficient framework by integrating experiment and multi-scale simulation (DFT/AIMD, phase-field model) for mechanism study in broad time and size scales.
- **Experiment:** Electrochemical characterization of state-of-the-art electrolytes to disclose thermodynamic information for feeding electrochemical modeling.
- **Electrochemical modeling:** Studied Faradaic efficiency dependence of cell performance (e.g., overpotential) and operation conditions.
- **DFT/AIMD:** Explored electronic density distribution, proton formation and migration in BZY and BCY based electrolyte materials.

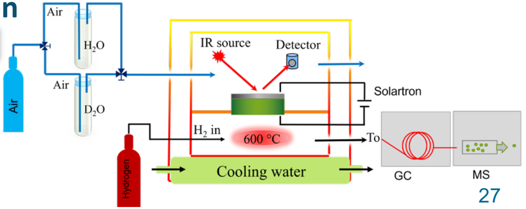


**Mechanism study**



**Operando proton conducting investigation**





# HydroGEN Lab R&D p-SOEC Technical Progress:

## Faradaic Efficiency Validation and Prediction, and Recommended Strategies for Higher Faradaic Efficiency

- **High accuracy in experimental data simulation**
  - Electrochemical performance under different operating conditions was simulated by electrochemical models.
  - The accuracy of the electrochemical simulation was validated using electrochemical experiment data.
  - Predictions of **extrinsic conditions** will help tune the experiment protocol.

**Successfully completed annual milestone by establishing multi-scale framework and validating its accuracy.**

- **Suggest effective strategies of boosting Faradaic efficiency**

➢ **Increase proton conductivity**

➢ **Decrease polarization resistance**

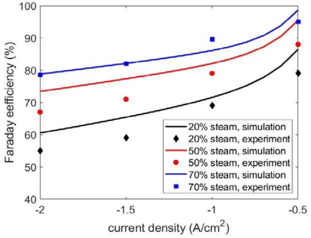
➢ **Optimize the operation conditions**

✓ Proper dopant and doping level

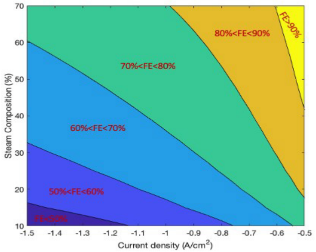
✓ High performance cell development

✓ Adopt the optimal operation conditions (e.g., temperature, steam concentration, etc.)

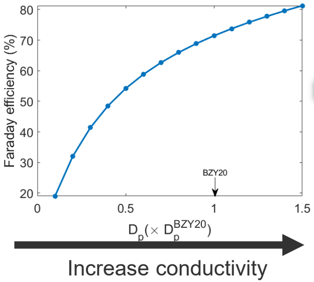
### Validate experiment data

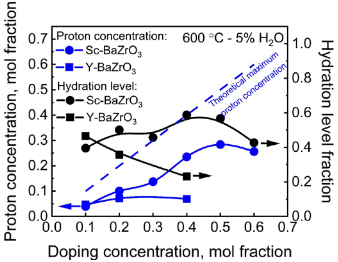


### Predict optimal conditions

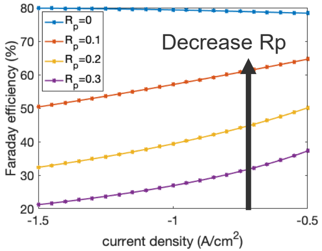


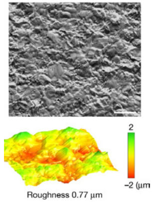
### New electrolyte material BZS developed with higher proton conductivity

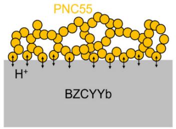




### New surface of electrolyte (acid etch) developed with lower overpotential



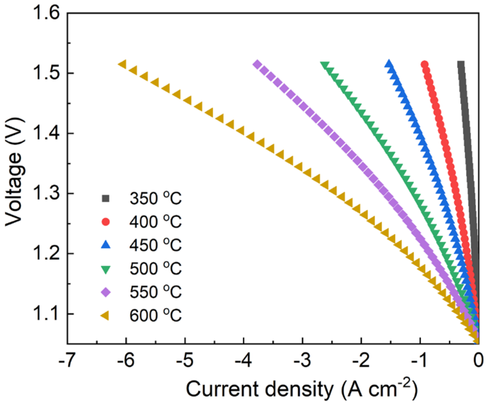


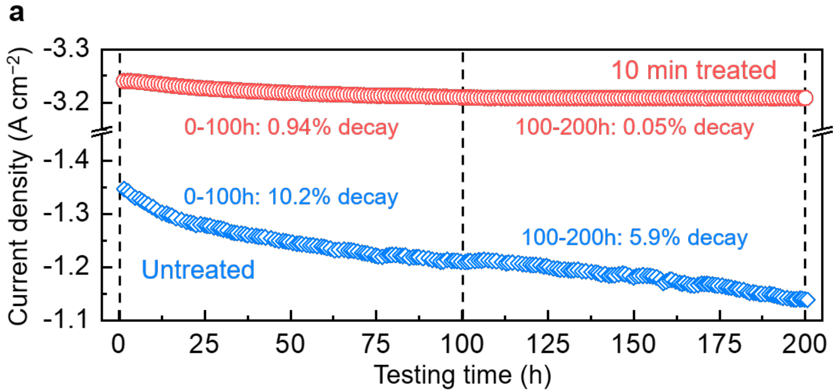


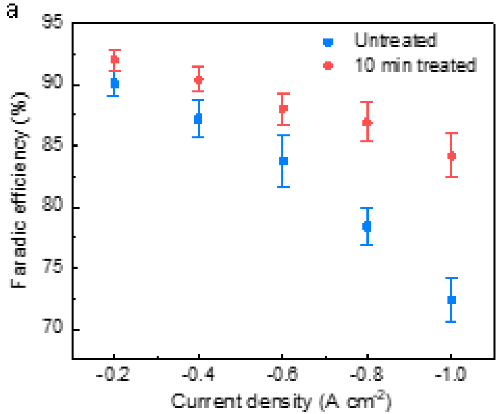
# Record performance of p-SOEC with smaller overpotential and lower operating temperatures

**High performance p-SOEC indicates not only cost reduction of materials and manufacturing for hydrogen production but the promotion of Faradaic efficiency.**

- Simple but scalable acid etching can significantly reduce both Ohmic and interfacial polarization resistance, thus improving the performance of p-SOEC (>2.8 A cm$^{-2}$ at 1.3 V @600$^o$C).
- Durability is also enhanced compared with the pristine cells.
- p-SOEC can maintain a reasonable performance @350$^o$C.
- Interface engineering represents a new direction for p-SOEC to bolster the performance and durability.
- Completed the GNG milestone by adopting the benchmarking electrolyte composition and further optimizing the operating conditions



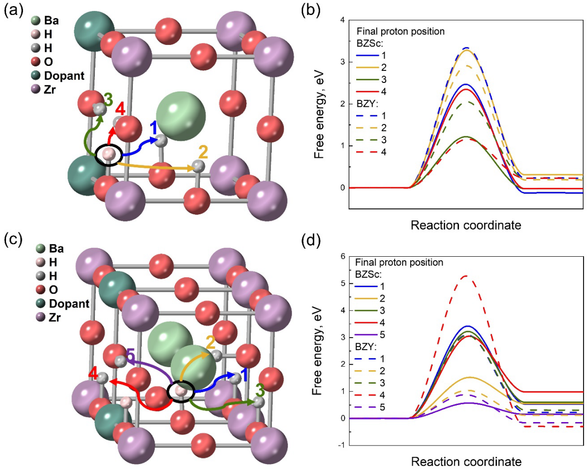


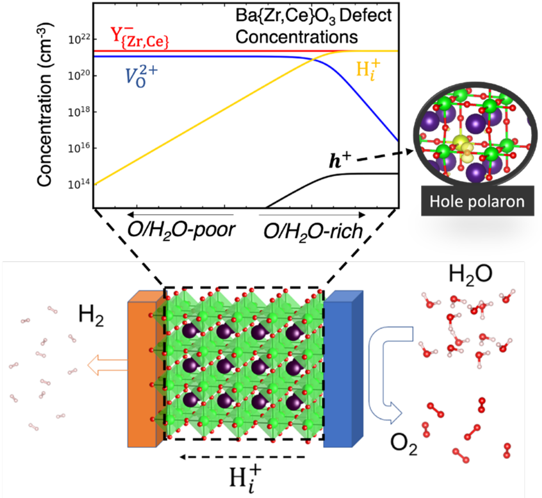


**W Bian, W. Wu, D Ding, et al. Nature, 2022**

# Proton Migration Mechanism and Source of Electronic Leakage in Doped $BaZrO_3$ Electrolytes
## HTE Lab R&D p-SOEC Accomplishments

- **Studying proton migration mechanism in doped $BaZrO_3$ electrolytes**
  - Mapped out proton migration pathways in Sc-doped $BaZrO_3$ (BZSc) in comparison to Y-doped $BaZrO_3$ (BZY) .
  - Discovered hydration level in electrolytes is a dominant factor governing proton diffusion energy.





- **Identified Source of Electrical Leakage in p-SOECs**

We showed that hole ($h^+$) polaron concentrations rise with $p_{O_2}/p_{H_2O}$ in Y-doped $BaZrO_3$. Reduce Y doping level, use $O_2/H_2O$-poor conditions to limit electrical leakage.

# LBNL Metal-Supported Solid Oxide Electrolysis Cell (MS-SOEC)

## HTE MS-SOEC Approach and Accomplishments

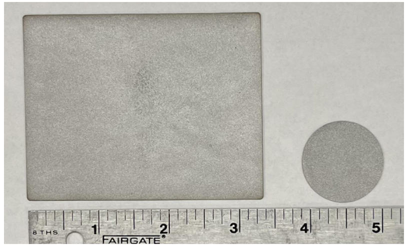
**FY23 targets (project end) at 700°C, 50:50 $H_2O:H_2$**

Performance
Target: > 1.0 A/cm$^2$ at 1.4V
Status: 1.2 A/cm$^2$ at 1.4V

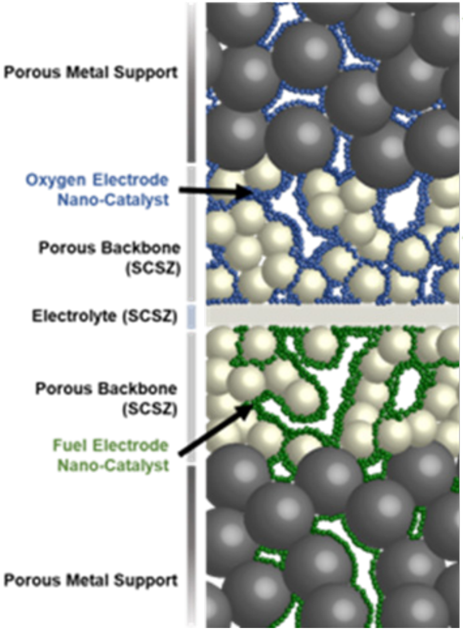
Durability
Target: <5%/kh
Status: 9%/kh at 0.5 A/cm$^2$

Cell size
Target: >40 cm$^2$
Status: 5 cm$^2$

**Large cell sintered, ready for catalysts**



**Approaches to improve performance and durability**



Protective coatings to block Cr

Catalyst composition and processing
- firing temperature
- Number of infiltration cycles
- Alternative OER catalysts
- Ni:SDC ratio
- Ni alloying

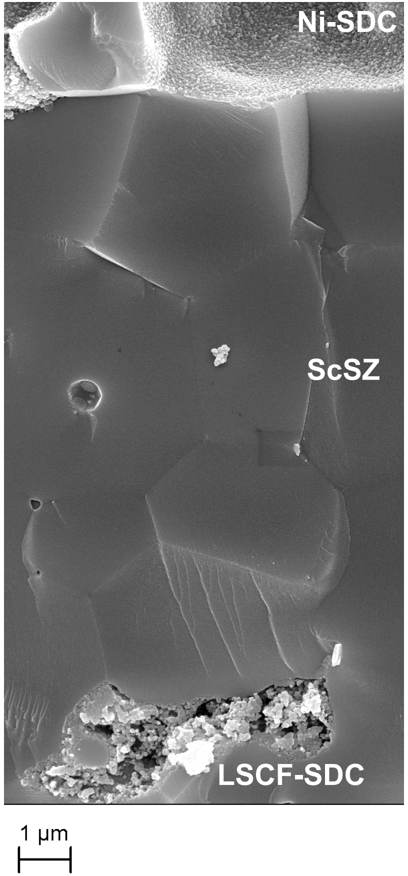
Cell structure and processing
- Support thickness and porosity

Operating conditions
- Temperature
- $H_2O:H_2$ ratio (high $H_2O$ utilization)
- Dry air

# MS-SOEC Optimization Examples

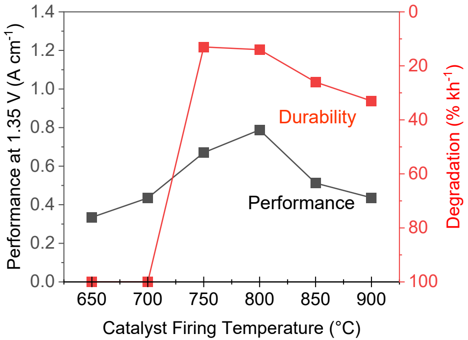
## HTE MS-SOEC Accomplishments

700°C, 50:50 $H_2O$:$H_2$



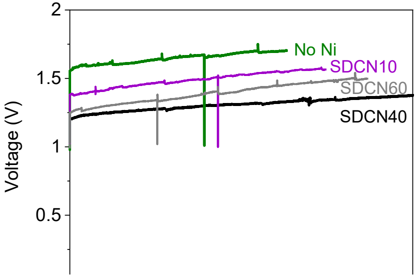
### Catalyst Firing Temperature

800°C firing improves performance and durability



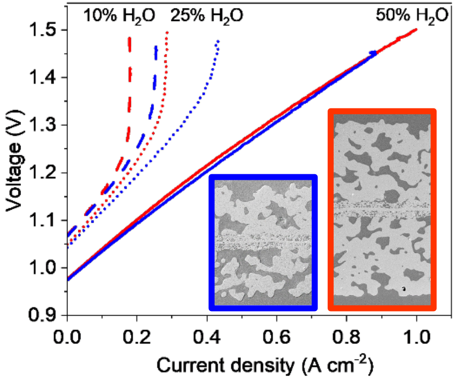
### Ni:Sn-Doped Ceria Ratio

40% Ni is optimum; 100% SDC (no Ni) is functional



### Metal support structure

Thinner, more porous support increases performance at low steam content



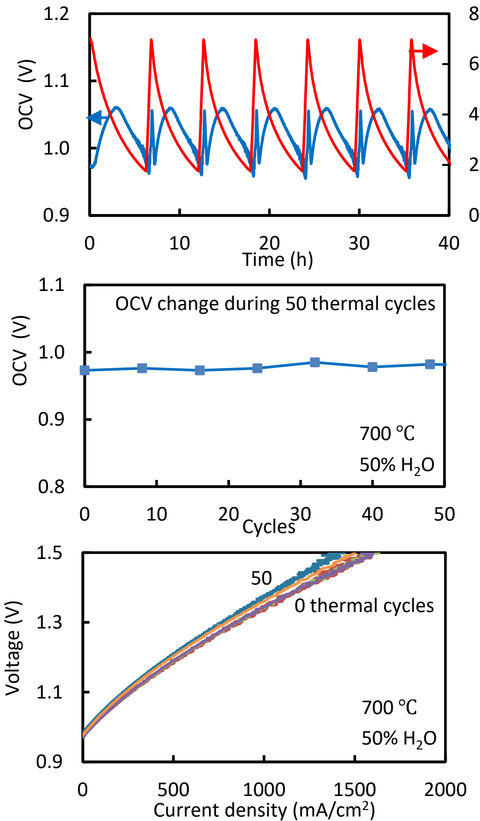
**Future work:**

- Optimize coating thickness, composition, uniformity, firing
- Continue catalyst development
- Detailed degradation mode analysis (DRT and post-mortem)
- Scale up to 40 $cm^2$ cell

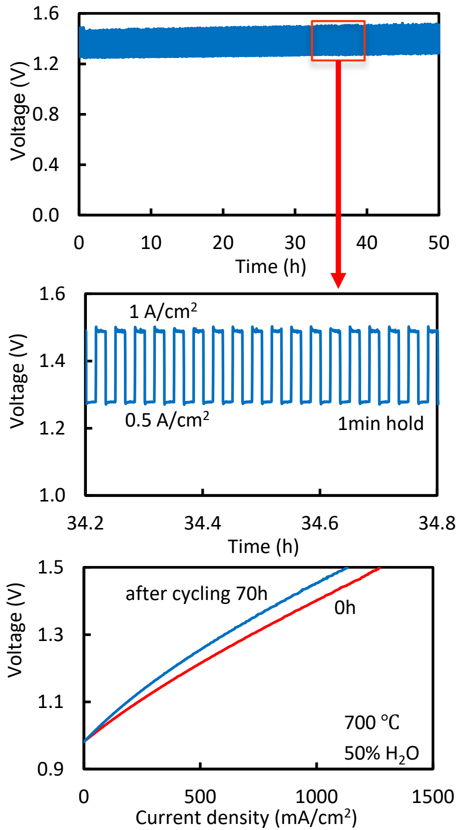
# HTE MS-SOEC Dynamic Operation

## HTE MS-SOEC Accomplishments

### Thermal Cycling



### Current Cycling



### Thermal Cycling (finished)

- 50 cycles from 160°C to 700 °C
- Stable OCV: no leaking
- Degradation rate less than constant temperature breaking-in: thermal cycling does not damage the cell

### Current cycling (on going)

- Different 1 min current cycles (0.5/0.8/1 A/cm$^2$)
- EIS and IV tracked every 70 h

### Redox cycling (future work)

- Cathode switching between $H_2/H_2O$ and Air

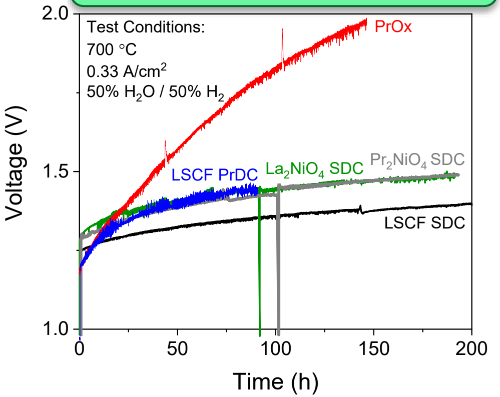
### Steam content cycling (future work)

- Cathode switching between Hi/Lo steam content

# HTE MS-SOEC: OER Catalysts and Protective Coatings

## HTE MS-SOEC Accomplishments

### Catalyst screening

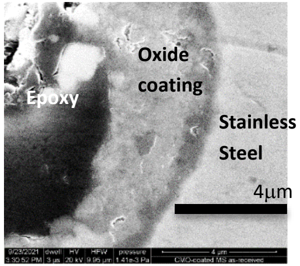

Test Conditions:
700 °C
0.33 A/cm$^2$
50% $H_2O$ / 50% $H_2$

**Selected:**
**LSCF/SDC 11x infiltrations**

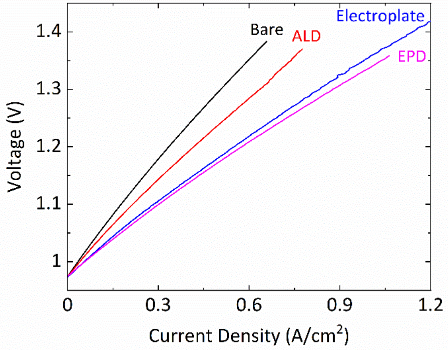
**Future work:**
- Optimize coating thickness, composition, uniformity, firing protocol
- Continue catalyst screening
- Optimize catalyst firing
  - higher temp to stabilize SDC-Ni
  - lower temp to avoid Cr on LSCF
- Scale up to 40 cm$^2$ cell

### Coatings

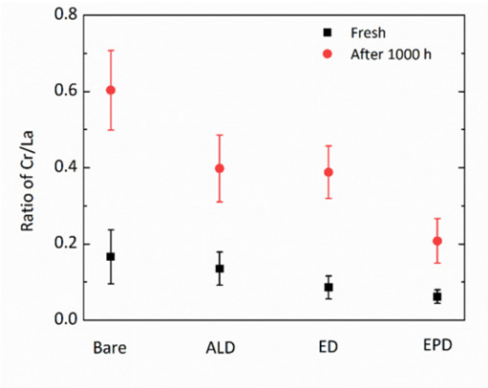
Coatings suppress Cr during cell fabrication (fresh) and after operation (1000h)



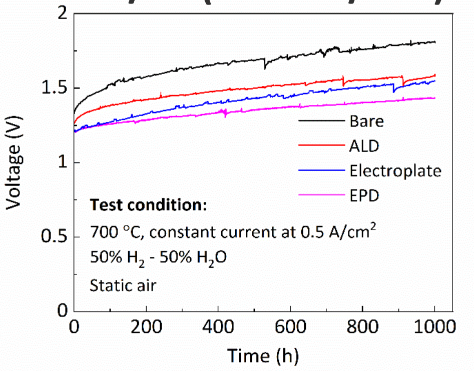
**1.2 A/cm$^2$ at 1.4 V**



**Cr in LSCF electrode**



**13 %/kh (at 0.5 A/cm$^2$)**


**Test condition:**
700 °C, constant current at 0.5 A/cm$^2$
50% $H_2$ - 50% $H_2O$
Static air

# HTE Accomplishments Summary and Proposed 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 demonstrated the high-performance p-SOEC with improved Faradaic efficiency, suggesting its potential in cost-saving and market adoption.
- **MS-SOEC Lab R&D**: Proven the enhanced durability of MS-SOEC by optimizing the coating, processing, cell configuration, and scaled up the cell size up to 40 $cm^2$

## Proposed Future Work:

- Continue leveraging the lab node support for the upcoming FOA projects.
- Benchmark and develop the new p-SOEC electrolyte materials that have higher proton conductivity, less electronic leakage, and better chemo-mechanical properties.
- Develop more robust and larger cells for MS-SOEC

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

# Low Temperature Electrolysis (LTE) Technical Accomplishments: Shaun Alia

## Participating Labs: NREL, LBNL, SNL

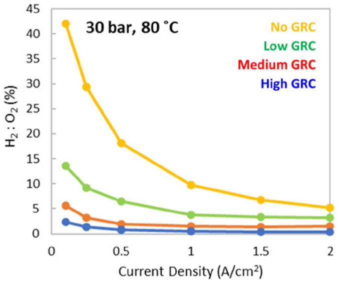
Project ID # P148A

# HydroGEN LTE Seedling Projects with Lab Capability Support

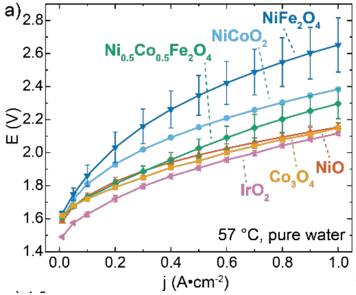
## Technical Accomplishment Highlights

- **(P185, GT, PP, USC, NEL and, NREL, LBNL, SNL) High-Performance AEM LTE with Advanced Membranes, Ionomers and PGM-Free Electrodes:** Minimized durability losses (30 µV/1000 hr at 1.77 V for 270 hr at 1 A/cm$^2$) and distinguished between degraded materials (catalyst, ionomer, PTL, AEM) and harmless conditioning of nickel, stainless steel, or other components.

- **(P186, Chemours, LANL, and NREL, LBNL) Performance and Durability Investigation of Thin, Low Crossover Proton Exchange Membranes for Water Electrolyzers:** Quantified effect of gas recombination catalyst (GRC) loading and identified membrane protrusion into the porous transfer layer (PTL) as potential risk factor for hydrogen crossover stability. Making GRC membranes more resistant to topographical changes has been a priority.



- **(P187, UO and NREL, LBNL, SNL) Pure Hydrogen Production through Precious-Metal-Free Membrane Electrolysis of Dirty Water:** Identified and characterized key degradation modes of AEM electrolysis in pure and contaminated water associated with ionomer oxidation at the anode and develop new catalyst and mitigation strategies for high performance and durability.



# Enabling High Efficiency, Durable AEM Electrolysis Performance

## LTE Lab R&D Goals and Approach

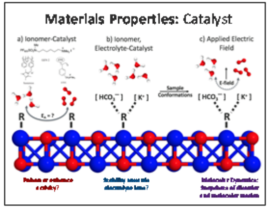
NREL Transforming ENERGY · BERKELEY LAB · Sandia National Laboratories · 5 Nodes

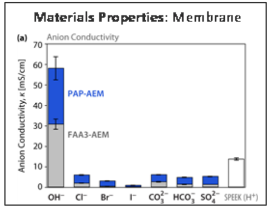
## Goals: Determine the role of the supporting electrolyte and the limiting factors behind water operation in AEM electrolysis

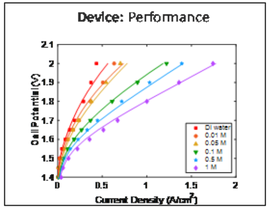
- Evaluate AEM's ability to approach PEM performance/durability
- Elucidate interactions at the ionomer/catalyst interface to assess ionomer stability and catalyst poisoning
- Understand the impact of catalyst layer composition on performance in a supporting electrolyte
- Delineate the impact of electrolyte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

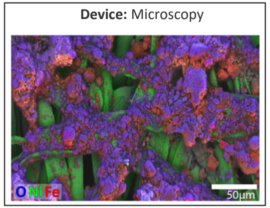
Materials Selection
- Electronic Structure Modeling (**NREL**)
- Ionomer Thin Films (**LBNL**)
- Microelectrodes (**LBNL**)
  - In-situ Cell Testing (**NREL**)
  - Microscopy (**SNL**)
  - Multiscale Model (**LBNL**)

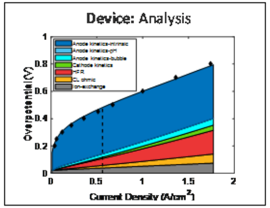
**Materials** → **Devices**


**Materials Properties:** Catalyst


**Materials Properties:** Membrane


**Device:** Performance


**Device:** Microscopy


**Device:** Analysis

# Effect of Dopants on Adsorption and Ionomer-Catalyst Interactions

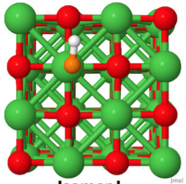
## LTE Lab R&D Accomplishments

### Doping NiO with Fe or Co *stabilizes* ionomer fragments, incl. ETFE/GEN 2’s tetramethylammonium

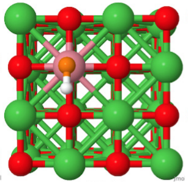
- Previous calculations showed that on NiO, *ETFE, GEN2 ionomers* are *unstable to demethylation* and *poison active sites*

- New calculations show that **adding Fe and Co *stabilizes tetramethylammonium fragment***

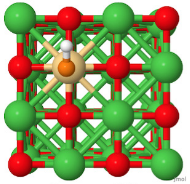
- OH* is *bound more strongly* on Fe- and Co-NiO



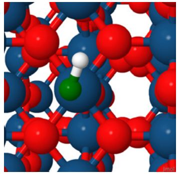
**Isomer I**
**$E_{OH}$ (ev) = -1.49**
Ni-OH* (atomic)



**Isomer I**
**$E_{OH}$ (ev) = -2.40**
Co-OH*



**Isomers I-II**
**$E_{OH}$ (ev) = -3.25 to -3.24**
Fe-OH*

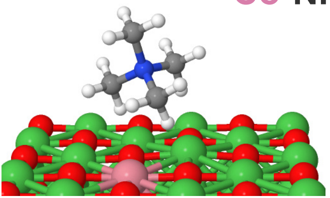


Isomer I
$E_{OH}$ (eV) = -3.72
Ir-OH*

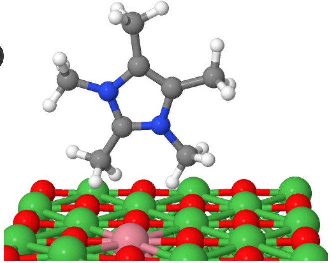
- ***OH* adsorption closer to $IrO_2$’s may increase activity***

**Co-NiO**

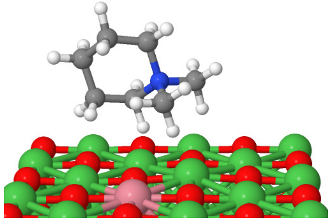
**I, $E_{ads}$ (eV) = -1.79**



**I, $E_{ads}$ (eV) = -1.45**

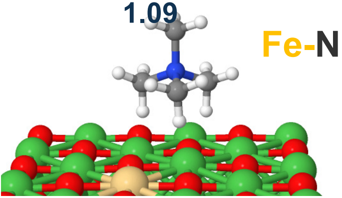


**I, $E_{ads}$ (eV) = -1.45**

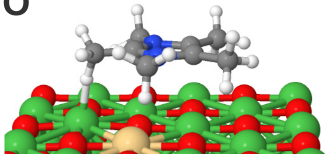


**Fe-NiO**

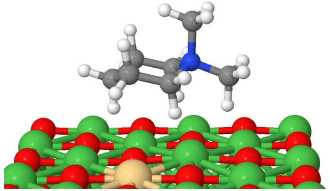
**I, $E_{ads}$ (eV) = -1.09**



**I, $E_{ads}$ (eV) = -0.74**



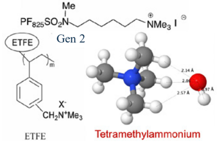
**I, $E_{ads}$ (eV) = -0.77**



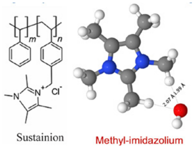
**ETFE/Gen 2 → Stable, Active Sites Available for OH**

**Sustainion → Stable, Active Sites Available for OH**

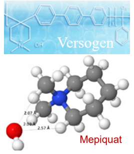
**Versogen → Stable, Active Sites Available for OH**



Tetramethylammonium



Methyl-imidazolium

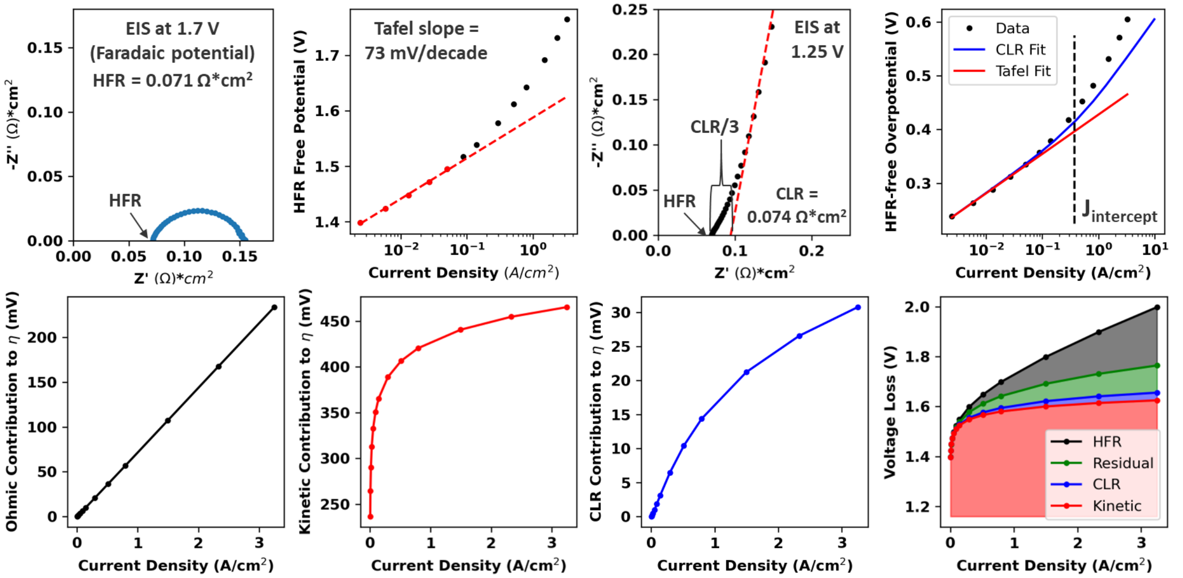


Mepiquat

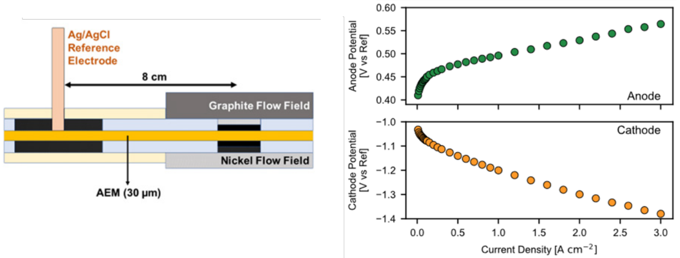
# Diagnostics and Resistance Analysis in Continuum Model

## LTE Lab R&D Accomplishments

High Frequency Resistance Determination → Tafel Slope Calculation → Catalyst Layer Resistance Determination → Voltage Loss Fitting



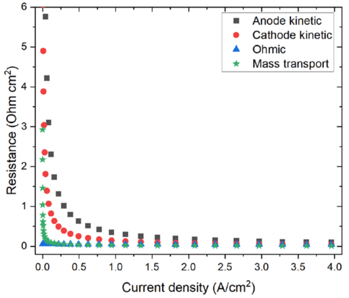
### Reference Cell



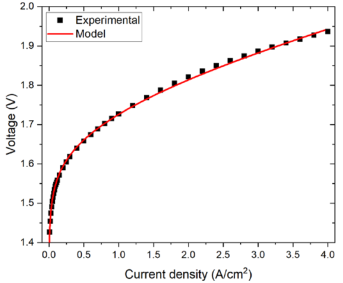
A. W. Tricker, et. al, " *Journal of Power Source* 567 (2023) 232967

Resistance analysis utilizes power-loss method

$$P = IV = I^2R \qquad \Delta V_k = \frac{\int_{V_k} \nabla\cdot \mathbf{p_k}\, dv_k}{I_{cell}} \qquad \Delta R_k = \frac{\int_{V_k} \nabla\cdot \mathbf{p_k}\, dv_k}{I_{cell}^2}$$



**The 1D continuum model successfully predicts experimental polarization curve**



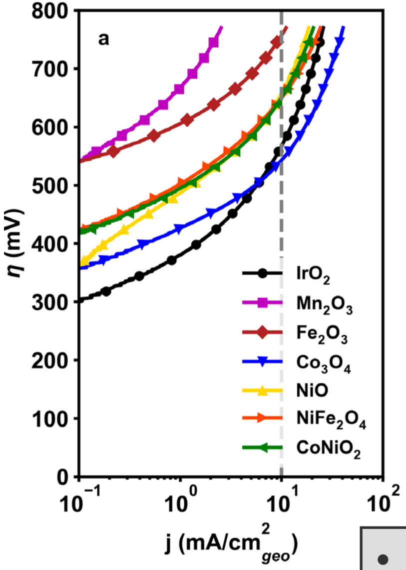
- Improved diagnostics to resolve catalyst layer resistance and anode/cathode contributions
- Suggests pathways for performance and durability improvements
- Agreement between diagnostics and continuum model

# Catalyst Screening for Oxygen Evolution Reaction (OER)

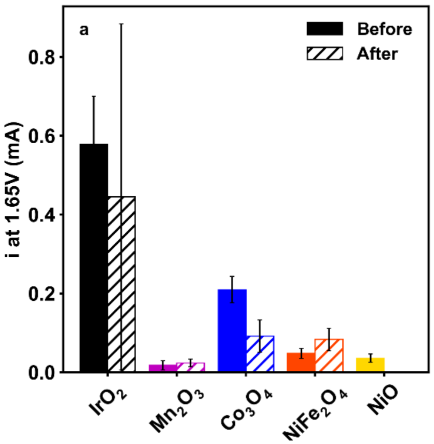
## LTE Lab R&D Accomplishments

### Ex-situ Materials Characterization

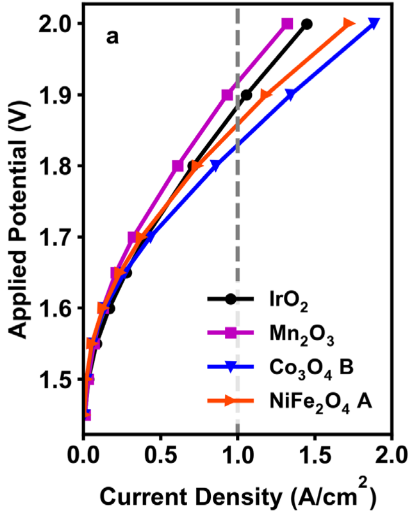
**Performance**



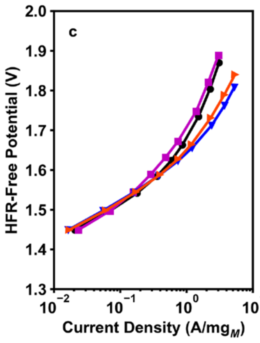
**Durability**



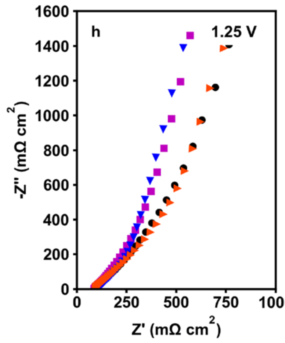
### Membrane Electrode Assembly (MEA) Testing



**HFR-free performance**



**Catalyst Layer Resistance**



5 cm$^2$ MEA in 1 M KOH,
Versogen (80 µm) membrane,
Versogen ionomer (30 wt%)

- Screened commercial catalyst materials for improved OER kinetics (RDE & MEA)
- PGM-free catalysts, nickel-iron ($NiFe_2O_4$) and cobalt ($Co_3O_4$) oxides, show promising OER activity: comparable to $IrO_2$
- $NiFe_2O_4$ OER activity improved after stress testing (13.5 h hold at 1.8 V), perhaps due dissolution of Fe and decrease in Fe content in spinel phase.

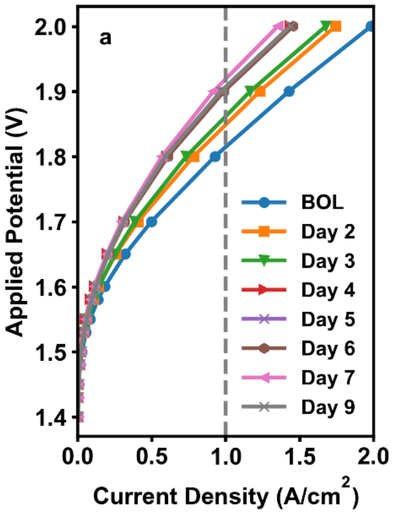
PGM: platinum group metal
RDE: rotating disk electrode

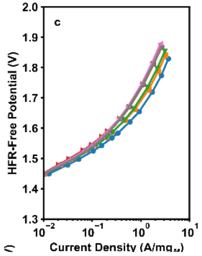
*Volk et al., Journal of the Electrochemical Society (2023) [Under Review]*

# Anode Catalyst Durability

## LTE Lab R&D Accomplishments

### $NiFe_2O_4$ Anode: 200 h operation





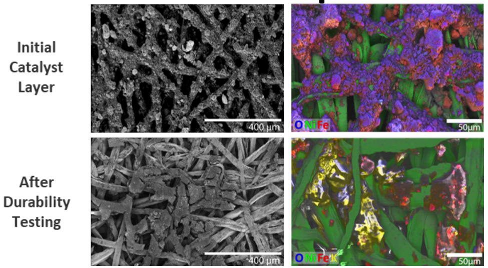
1 M KOH at 80°C

Versogen piperion TP85 membrane & ionomer

Anode: NiFe2O4 (30 wt% ionomer)

Cathode: Pt/C (30 wt% ionomer)

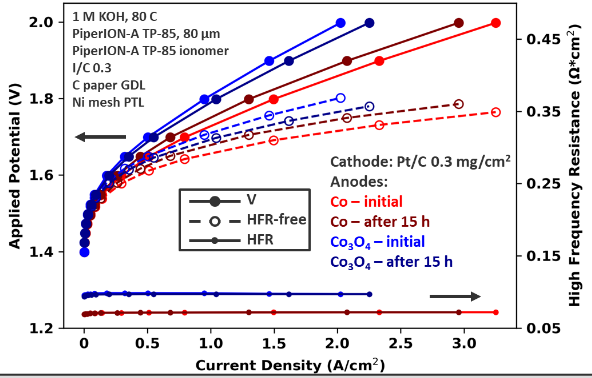
### 500 h operation



- 36% of performance loss after 200 h operation
- Observed iron loss during extended operation (500 h)

*Volk et al., Role of the Ionomer Anion Exchange Membrane Electrolyzers with Supporting Electrolyte [In Preparation]*

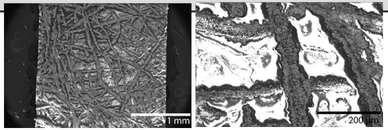
### Co Anode: 15 h operation



- After 15 h operation, Cobalt oxide ($Co_3O_4$) performance improves due to a decrease in catalyst layer resistance
- Cobalt metal performance decreases slightly, due to a decrease in number of active sites and site-specific activity
- After 400 h testing, catalyst layer transferred from PTL and embedded in the membrane, potentially affecting the integrity of membrane. Minimal catalyst layer compositional change

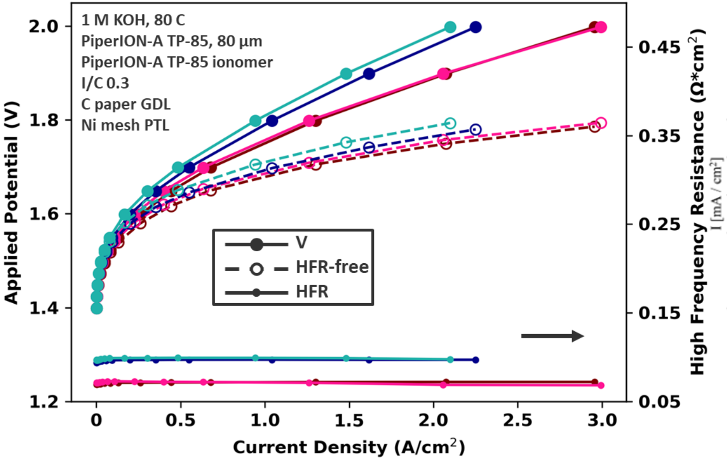
**400 h operation:**

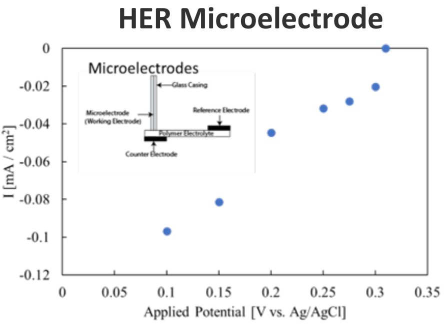
Cobalt oxide ($Co_3O_4$) Catalyst Layer, After Durability Testing

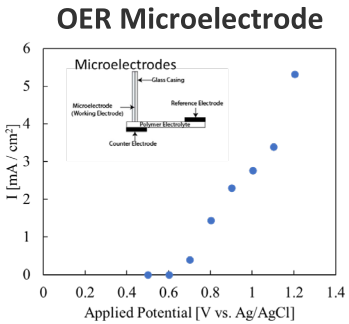


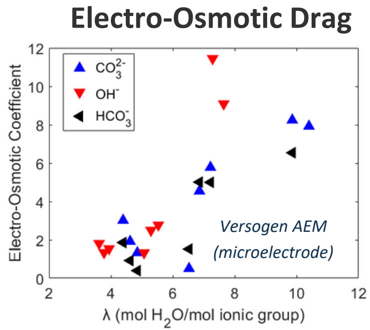
# Cathode Water Consumption and Effects of Dry Operation

## LTE Lab R&D Accomplishments

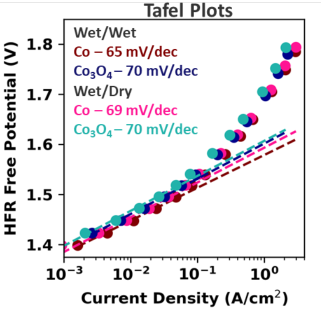








| | HFR (Ohm*cm²) | CLR (Ohm*cm²) | Tafel (mV/dec) |
|---|---|---|---|
| Co wet/wet | 0.072 | 0.072 | 65 |
| Co wet/dry | 0.071 | 0.073 | 69 |
| $Co_3O_4$ wet/wet | 0.096 | 0.239 | 70 |
| $Co_3O_4$ wet/dry | 0.096 | 0.345 | 70 |

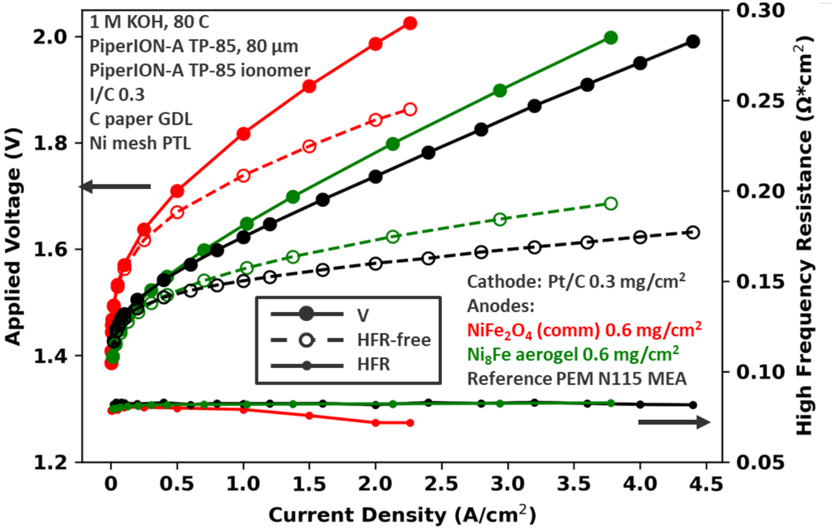


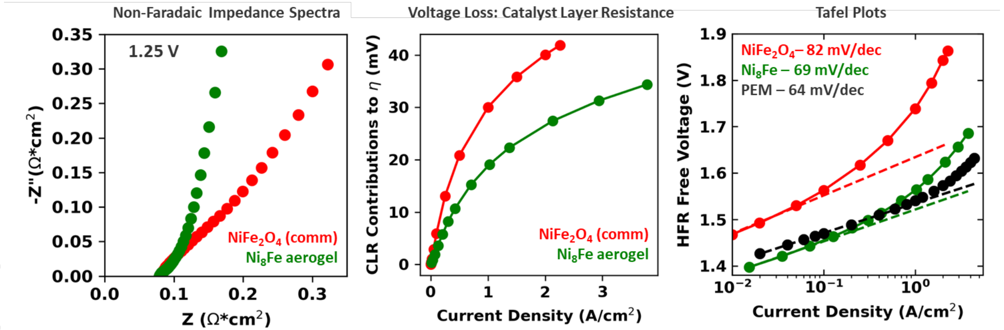
- Cathode is a larger concern in anion exchange membrane (AEM) electrolysis:
  - Kinetics and transport are factors
  - Poor catalyst-ionomer interaction at the hydrogen electrode (microelectrode)
- Feeding electrolyte to the anode simulates backpressure and requires transport across the membrane to the cathode (electro-osmotic drag)
- **Anode only feed has minimal effect on initial performance for Co and $Co_3O_4$ catalysts**

# Progress Towards LTE Performance Milestone of PGM-free OER Catalyst

**Accomplishment**

*__Milestone (9/30/2023):__ LTE Catalyst Testing in AEM MEA. __Criteria:__ Incorporating ElectroCat-developed catalysts, demonstrate cell overvoltage reduction of more than 50 mV (HFR-free) compared to commercial baseline catalysts (NiFeOx, established in HydroGEN EMN) at 1 A/cm². Comparisons between novel and commercial catalysts would maintain consistent supporting electrolytes (1 M KOH) and operating conditions, including materials choices, flow configurations (wet/wet), and temperature (80 °C).*





| System | HFR (Ω cm²) | CLR (Ω cm²) | Tafel (mV/dec) | $V_{HFR\text{-}free}$ (V) at 1.0 A cm$^{-2}$ |
|---|---|---|---|---|
| **$NiFe_2O_4$** | 0.078 | 0.197 | 82 | **1.739** |
| **NiFe 8:1** | 0.082 | 0.078 | 69 | **1.559** |
| **PEM 115 MEA** | 0.083 | 0.008 | 64 | **1.541** |

- **Highlight: ElectroCat FY23 annual milestone exceeded by 130 mV with NiFe 8:1 catalyst** (1.559 V *vs.* 1.739 V baseline established with $NiFe_2O_4$ catalyst)
- **Highlight**: By reaching *HFR*-free voltage of 1.559 V NiFe 8:1 catalyst also met the **HydroGEN FY23 Q4 milestone**: *"Demonstrate AEMWE in a supporting electrolyte with a cell overvoltage within 50 mV (HFR-free) of commercial Nafion at 1 A/cm²"*. (*HFR*-free voltage for NiFe 8:1 catalyst is within 18 mV of the PEM 115 MEA performance.)

# LTE Accomplishments Summary and Proposed Future Work

## Summary:

- Doping nickel oxide (NiO) with cobalt, iron can both stabilize ionomers and enhance OH* adsorption, comparable to iridium oxide ($IrO_2$), potentially increasing catalyst durability and oxygen evolution activity
- Screening of commercial materials improved membrane electrode assembly kinetics to approach technology target
- Incorporated diagnostics that improved resolution of loss type and cause. Materials challenges including balancing site-access and mechanical integrity, catalyst/transport layer conductivity and passivation, and nonideal interfacial contact, all affect performance of the technology.

## Proposed Future Work:

- Lab R&D:
  - Optimize catalyst layer composition and processing technique to improve site-access, catalyst layer resistances, and device performance
  - 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
- Leverage HydroGEN nodes to enable successful completion of current and new seedling projects.

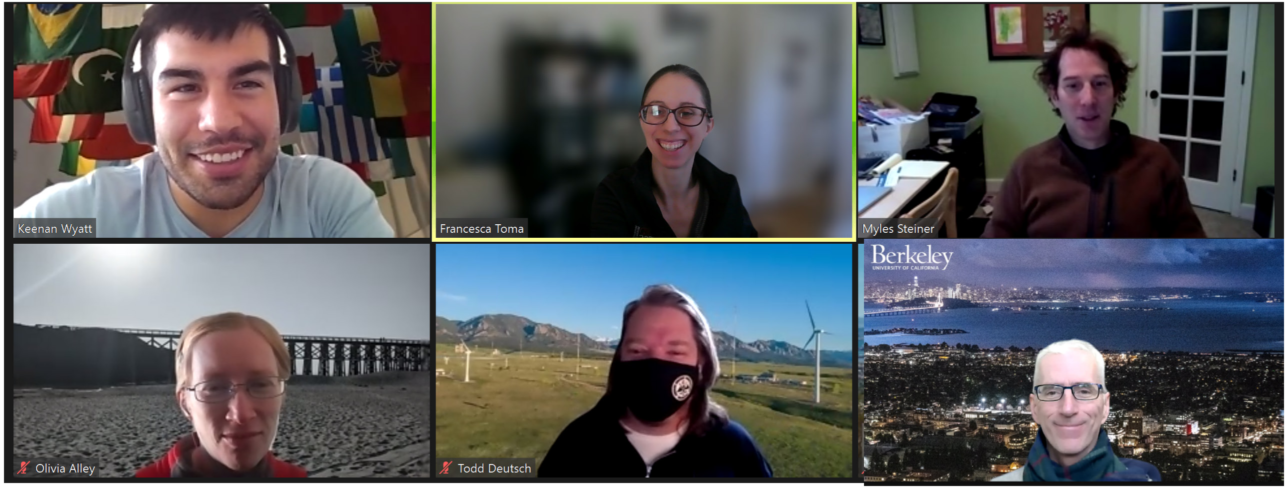
Any proposed future work is subject to change based on funding levels

# Collaboration, Effectiveness

- Interfacing between HydroGEN and IEA Annex 30 in benchmarking
- Interfacing between HydroGEN and ElectroCat in catalyst benchmarks
- Contributions to the Meta Data development for the HydroGEN Data Center

| Seedling Leads | Seedling Teams | LTE 2.0 Team | |
|---|---|---|---|
| Shannon Boettcher<br>Paul Kohl<br>Andrew Park | Chemours<br>PAJARITO POWDER FUEL CELL CATALYSTS<br>ADVENT<br>nel<br>Argonne NATIONAL LABORATORY<br>OAK RIDGE National Laboratory<br>Los Alamos NATIONAL LABORATORY EST. 1943<br>UNIVERSITY OF OREGON<br>UCIRVINE<br>Georgia Institute of Technology<br>Rensselaer<br>Northeastern University<br>UofSC South Carolina<br>University at Buffalo The State University of New York<br>UNIVERSITY OF DELAWARE | NREL Transforming ENERGY<br>Shaun Alia<br>Ai-Lin Chang<br>Huyen Dinh<br>Mai-Anh Ha<br>Melissa Kreider<br>Ross Larsen<br>Doug Marsh<br>Bryan Pivovar<br>Meital Shviro<br>Emily Volk | BERKELEY LAB Bringing Science Solutions to the World<br>Grace Anderson<br>Tugrul Ertugrul<br>Johnny Petrovick<br>Andrew Tricker<br>Xiong Peng<br>Adam Weber<br>Sandia National Laboratories<br>Josh Sugar |

# Photoelectrochemical Water Splitting (PEC): Joel W. Ager (March 2023-present), Francesca Toma (to March 2023)



## Participating Labs: LBNL, NREL, LLNL

**Not in the picture:**

- **James Young (NREL)**
- **Alex King (LBNL)**
- **Adam Weber (LBNL)**
- **Ethan Crumlin (LBNL)**
- **Rebecca Hamlyn (LBNL)**
- **Anh Pham (LLNL)**
- **Tadashi Ogitsu (LLNL)**

**Alumni:**

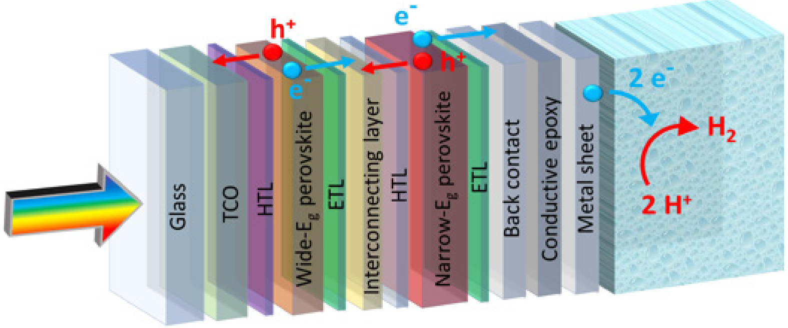
- **Guosong Zeng – Assistant Professor at Sustech**
- **David Larson – Twelve (Senior Prototyping Engineer)**
- **Guiji Liu – eJoule International (Senior Scientist)**

Project ID # P148C

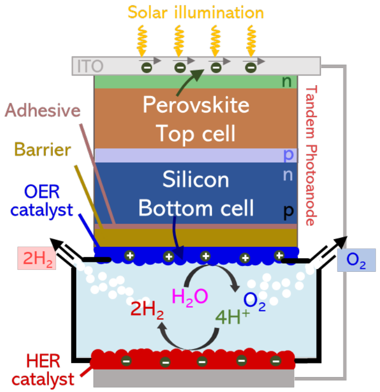
# HydroGEN PEC Seedling Projects with Lab Capability Support

## Technical Accomplishment Highlights

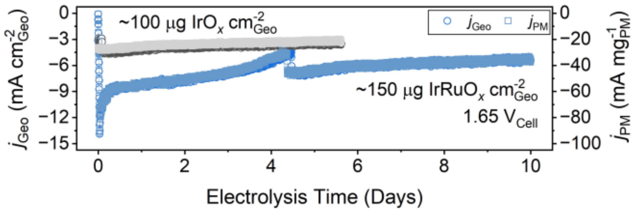
- (P191, U. Toledo, NREL) All-perovskite tandem photoelectrodes for unassisted solar hydrogen production: Perovskite/perovskite tandem photoelectrodes deliver an unbiased STH >18% in a two-electrode configuration under one sun illumination for more than 500 hours.

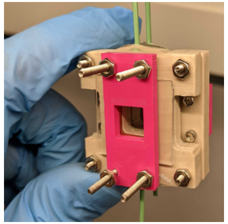


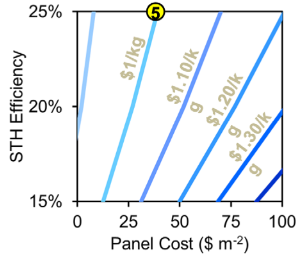
- (P193, Rice, NREL, LBNL) Integrated halide perovskite photoelectrochemical cells with solar-driven water-splitting efficiency of 20.8% : Use of corrosion resistant barrier layers including hydrophobic polymers and ALD oxides enables >100 hours of continuous 1-sun operation at STH > 20%.



Towards earth abundant OER catalysts



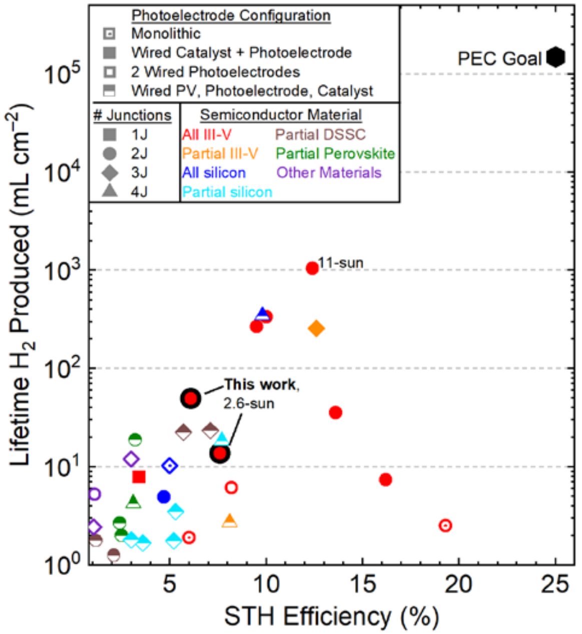




# HydroGEN PEC Lab R&D Goal and Approach

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

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



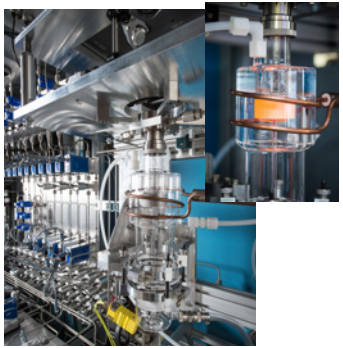
*Comparison of the solar to hydrogen efficiency (STH) and lifetime H2 produced for unassisted water splitting devices. The "PEC Goal" point in the upper right was calculated assuming a 20% capacity factor over a 10 year lifetime (15) .*

## Approach:

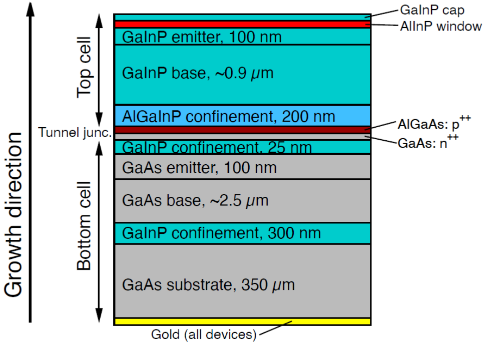
- Prioritize durability stressors and establish PEC device durability protocol
- Use density functional theory (DFT) and microkinetic modeling to describe the local environment at the electrode/electrolyte interface under operation
- Provide mechanistic understanding of PEC device degradation guided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

# HydroGEN PEC Lab R&D Technical Progress

## Photoelectrode growth by metal organic vapor phase epitaxy (MOVPE)



*MOVPE at 620℃ growth temperature*

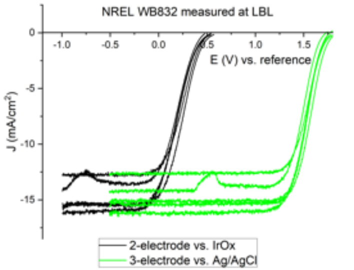


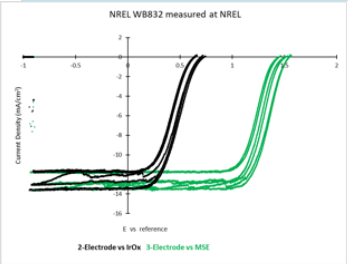
*Schematic of the III-V high efficiency photoelectrode*

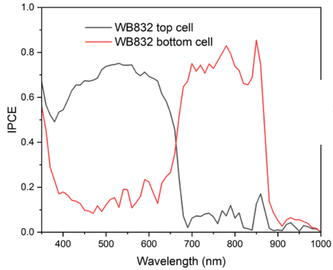
## Photoelectrode Fabrication and Testing at NREL and LBNL

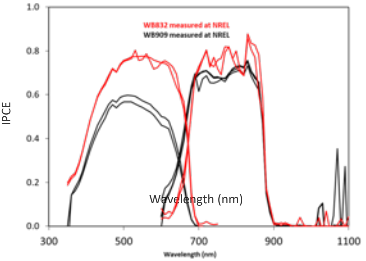
*Dual anode cell with high modularity and ease of fabrication*

***Reproducibility achieved at both Labs***

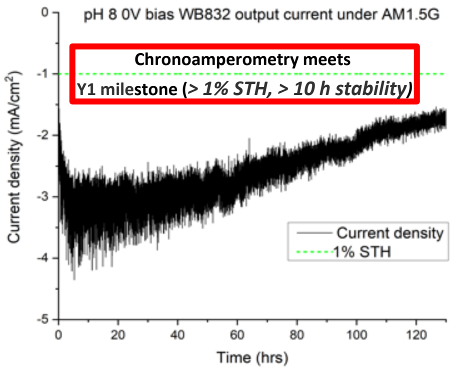




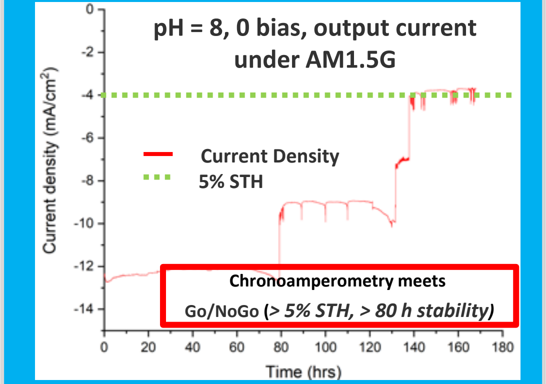




## Progress to Date



**Chronoamperometry meets Y1 milestone (*> 1% STH, > 10 h stability*)**



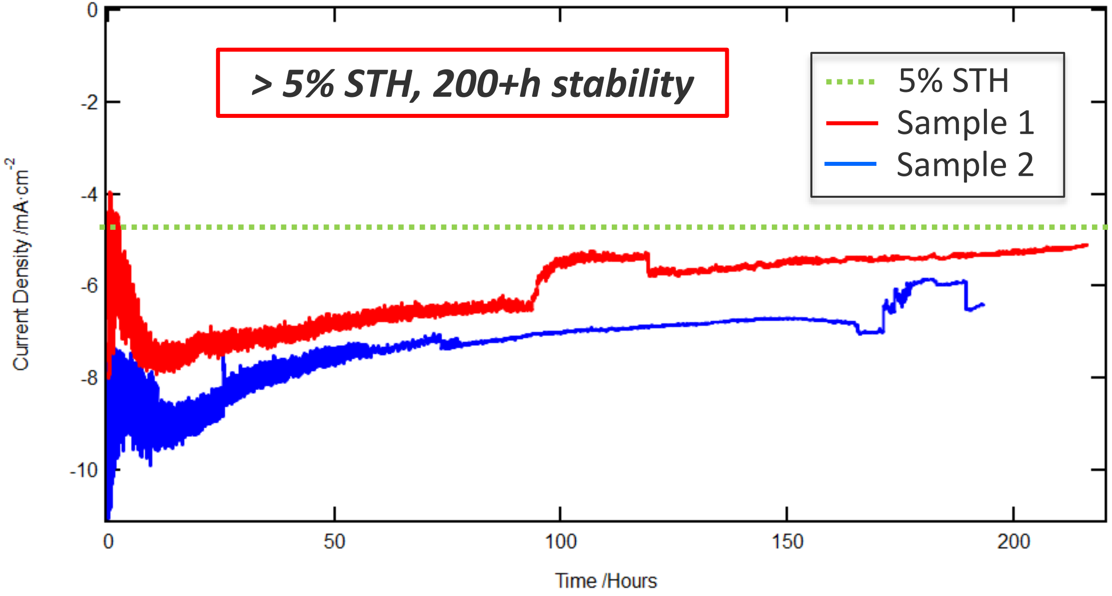
**Chronoamperometry meets Go/NoGo (*> 5% STH, > 80 h stability*)**

# Progress towards Q4 milestone

## PEC Lab R&D Accomplishment

**Annual milestone (FY23Q4)**: *Demonstrate a completely integrated system and neutral pH conditions that achieve >220 h durability at short circuit and > 5% STH efficiency.* Scale-up to a hand-held >4 $cm^2$ active area device that will split water under direct sunlight illumination with appreciable hydrogen bubble generation.

***Bias-free water splitting at neutral pH in cuvette cell***



**Chronoamperometry shows significant progress towards Q4 milestone**

***Cathode:*** *two electrodes from growth # WC106 of GaInP/GaAs III-V tandem, with PtRu catalyst*
***Cathode active area:*** *0.2 $cm^2$*
***Anode****: IrOx, separated from the photocathode via Ti mesh*
***Electrolyte****: pH 7.2 potassium phosphate remains at neutral pH in bulk throughout 200 hours*
***Measurement vessel****: cuvette cell*

# Impactful standard protocol and benchmarking publication

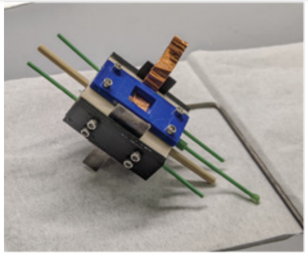
## PEC Lab R&D Accomplishment

### *Best Practices in PEC Water Splitting: How to Reliably Measure Solar-to-Hydrogen (STH) Efficiency of Photoelectrodes*[1]

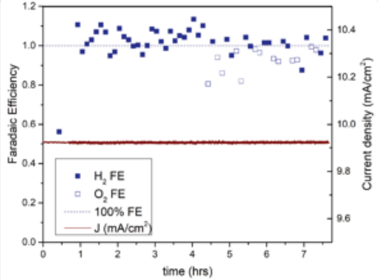
- Publication shares with PEC community best practices when measuring and reporting STH efficiency of new photoelectrodes and will improve the reproducibility of results across the field.

  *"This is a great paper for the community, thank you for dedicating the time to put this together, especially during this challenging historical time (pandemic)"*

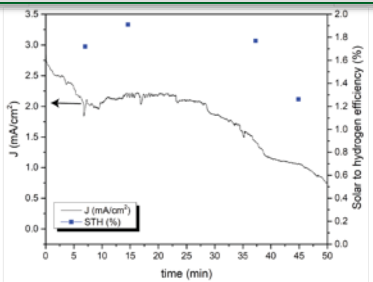
  *–2023 attendee, Solar Fuels Gordon Conference*
- Publication benchmarks a flow reactor for $H_2/O_2$ measurement, that any lab can produce from readily available materials using a CNC miller and 3D printer.
- 4098 views, 491 downloads, 10 mentions in news articles (4/10/2023)



**Reactor**



**Validation: dark Faradaic Efficiency**



**STH of III-V tandem at pH 0.4**

[1] *Front. Energy Res., 27 October 2022 Volume 10 - 2022 | https://doi.org/10.3389/fenrg.2022.884364*

# Impactful Publication: *Best Practices in PEC Water Splitting: How to Reliably Measure Solar-to-Hydrogen Efficiency of Photoelectrodes*

**PEC Lab R&D Accomplishment**

**A methodical approach**: We provided an in depth, step-by-step description of each factor that goes into the solar to hydrogen efficiency calculation.

## 2-electrode current density

Description of an accurate measurement of the photoelectrode area

## Quantification of $H_2/O_2$

Detailed protocol for quantification of $H_2$ and $O_2$ by gas chromatography (GC)

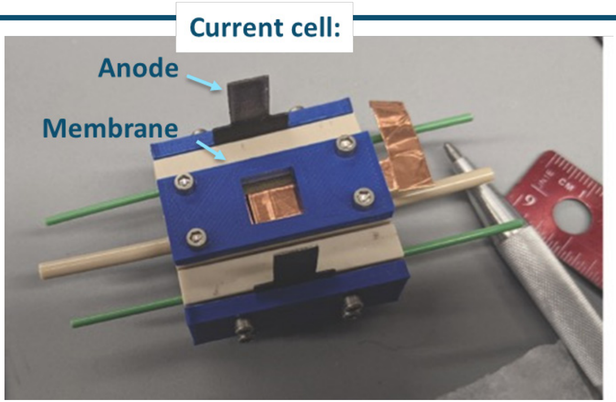
$$\eta_{STH} = \frac{j_{sc}\left(\frac{mA}{cm^2}\right) * 1.23V * \eta_{FE}}{P_{total}\left(\frac{mW}{cm^2}\right)}$$

## AM1.5G source calibration

Step-by-step procedure for solar simulator calibration that accounts for the current-limiting junction of a tandem photoelectrode

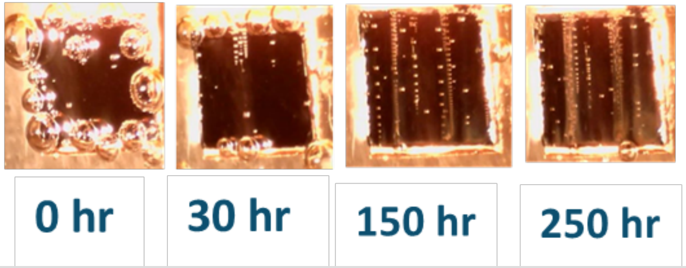
# Improving PEC cell design and Understanding III-V lifetime and durability

## PEC Lab R&D Accomplishment



**Future cell: Replace separate Ir/IrOx anodes with Ir CCMs**

**Evolution of photocathode at zero bias under illumination (III-V with GaP capping layer):**



- III-V water-splitting photoelectrodes have short lifetimes in 0.5 M $H_2SO_4$ (pH 0.4). Resistance due to ion transport is high at neutral pH
- To decrease resistance in neutral pH, the 0.5 cm ionic transit path from anode to membrane will be eliminated by merging anode and membrane into catalyst-coated membrane (CCM).
- Will allow bias-free water splitting at neutral pH in this cell

- Increased roughness of III-V surface following durability tests is thought to be from photoreduction and electrodeposition of Ga and In metal
- Increased roughness leads to more bubble nucleation sites on surface over time
- Will explore capping layers and protective layers to improve III-V lifetime

# PEC Accomplishments Summary and Proposed Future Work

**Summary:**

- Met Y1, Y2 and the Go/No Go milestones (5% STH efficiency with 50 h or better durability).
- Progressing towards PEC annual milestone (5% STH efficiency with > 220 h durability; *hand-held > 4 $cm^2$ device*).
- Gaining insights on degradation mechanisms and cell design
- Published impactful protocol in a special issue of *Frontiers in Energy Research Journal*.

**Proposed Future Work:**

- Achieve the "end of the project milestone":
  - Finalize geometry (aspect ratio) and PV strategy for handheld device
  - Modifying the reactor to use catalyst-coated membranes
  - Evaluate longevity of catalyst coated membranes in the context of durability goal
- Improve III-V lifetime and durability
  - GaN or GaP capping layer
  - $TiO_2$ or $Al_2O_3$ protective layers
  - use pre-post analysis to further study corrosive mechanisms
- Finalize a manuscript on benchmarking the cell used in HydroGEN 2.0 to provide the community a reliable cell for PEC testing.

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

Project ID # P148E

# Cross-Cutting Modeling

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

**Goal:** Exploit similarities in technical challenges across AWS technologies and required simulation capabilities to advance material performance and durability.

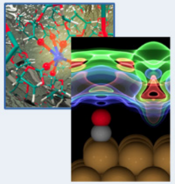
## Multiscale performance and durability modeling across the technology areas

| | Limiting factor | PEC | LTE | HTE | STCH |
|---|---|---|---|---|---|
| Performance | Materials thermodynamics | | | X | X |
| | Carrier generation and mobility | X | X | X | |
| | Interfacial (electro)chemical kinetics (solid-solid = S, solid-liquid = L) | L | L | S | |
| | Mass transport kinetics (solid = S, liquid = L) | L | L/S | S | S |
| | Phase transformation kinetics | | | X | X |
| | Multiphysics device operation | X | X | X | X |
| Durability | Thermomechanical | | | X | X |
| | Electrochemical | X | X | X | |
| | Photochemical | X | | | |

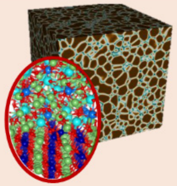
The modeling and simulation strategy will focus on key factors limiting performance and durability across the four advanced water splitting technology areas.

## Priorities for Cross-Cut Modeling Activities

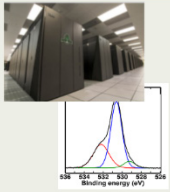
Materials under operando conditions



Multiscale integration



Experiment-theory feedback



***Theory-guided design:*** models and experimental testing will be combined to analyze performance and durability of the materials under simulated operating conditions. Sensitivity analysis will be utilized to connect the material properties (composition, microstructure, etc.) and operating environment (temperature, pressure, solution composition, current density) to device behavior.

## Pushing low-TRL technologies to higher TRL by:

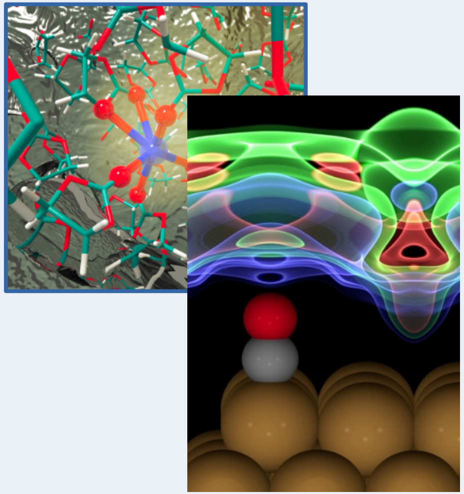
1. **Predictive simulations:** develop and apply multi-scale modeling capability to simulate performance and durability

   Provide clear link between material property and device performance/durability: crucial information for improving the component materials and their assembly
2. **Validation:** theory-experiment integrated approach to ensure reliability of simulation results and interpretation of experiments
3. **Sharing:** help develop accessible energy materials database for scientific community and industry
4. **Collaboration with H2NEW:** assist further advancement of high-TRL hydrogen production technologies (PEME, o-SOEC)

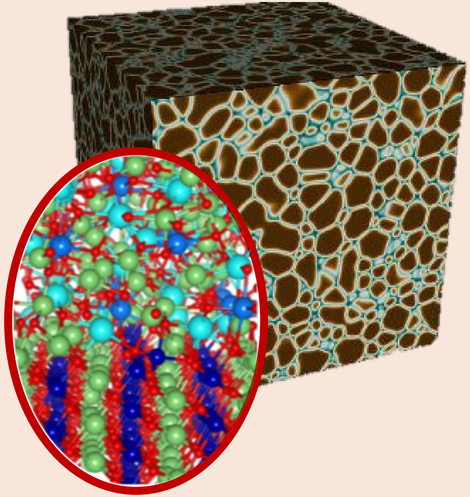
**The funding allocated to achieve this task is provided under other technology specific tasks.**

# Priorities for cross-cutting modeling activities

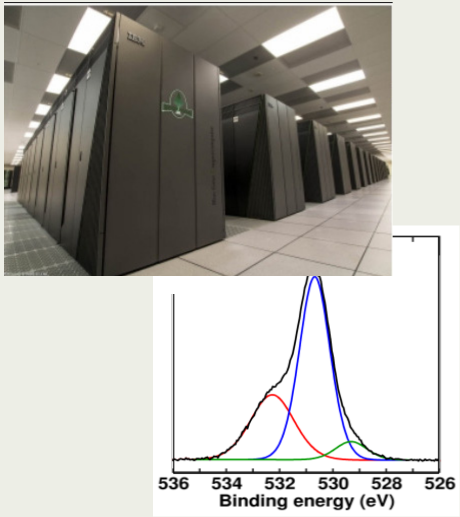
## Materials under operando conditions



## Multiscale integration

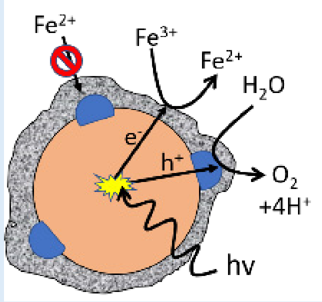


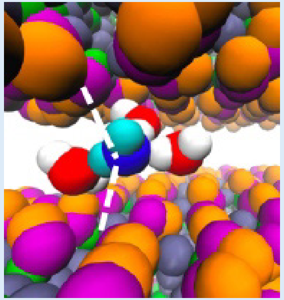
## Experiment-Theory-Data integration

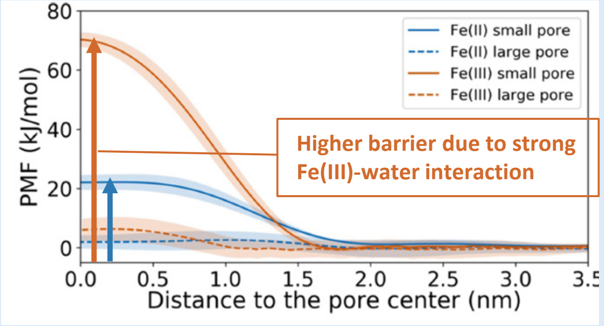


# Accomplishments of low-temperature technologies (PEC/LTE)
## Atomistic insights into transport, OER activities, stability

### **PEC:** Simulations demonstrate the ability to manipulate pore sizes and chemistry for selective hydrogen production.





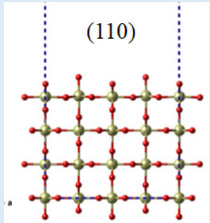


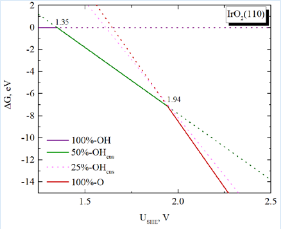
Higher barrier due to strong Fe(III)-water interaction

UCI seedling, ACS Appl. Mater. Interfaces, doi:10.11021/acsami.2c22865

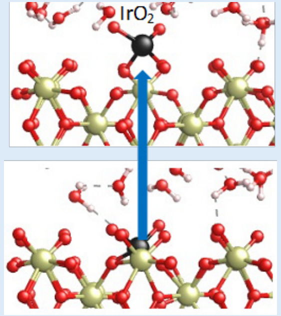
### **LTE:** Establish framework for modeling energetics of OER activities & stability of powder $IrO_2$

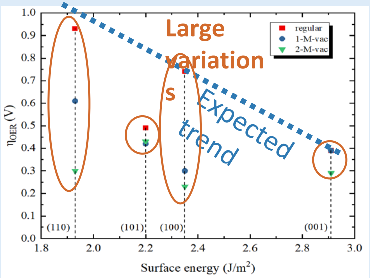
Pourbaix diagram of different surfaces. (110) is shown.





Correlating Ir dissolution and OER kinetics on different surfaces with and without defects





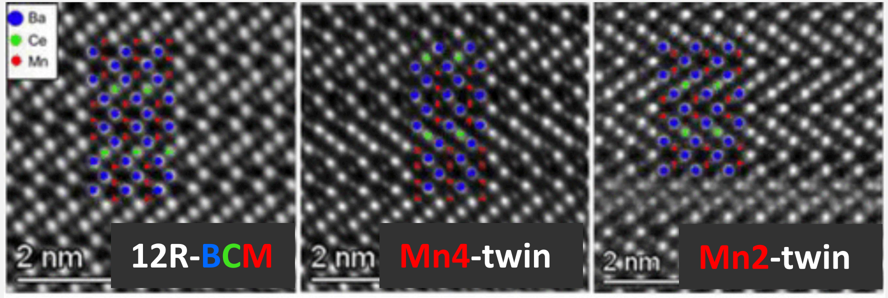
Large variations

Expected trend

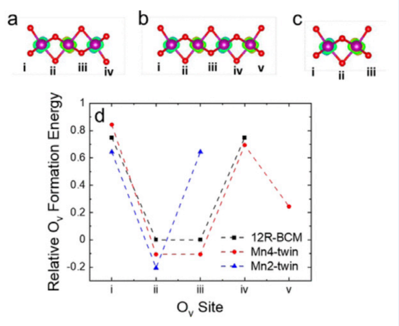
Paper in preparation

# Accomplishments of high-temperature technologies (STCH/HTE)
# Understand stability/role of defects at operation condition

## STCH: Phase change under operation condition



HAADF-STEM by SNL

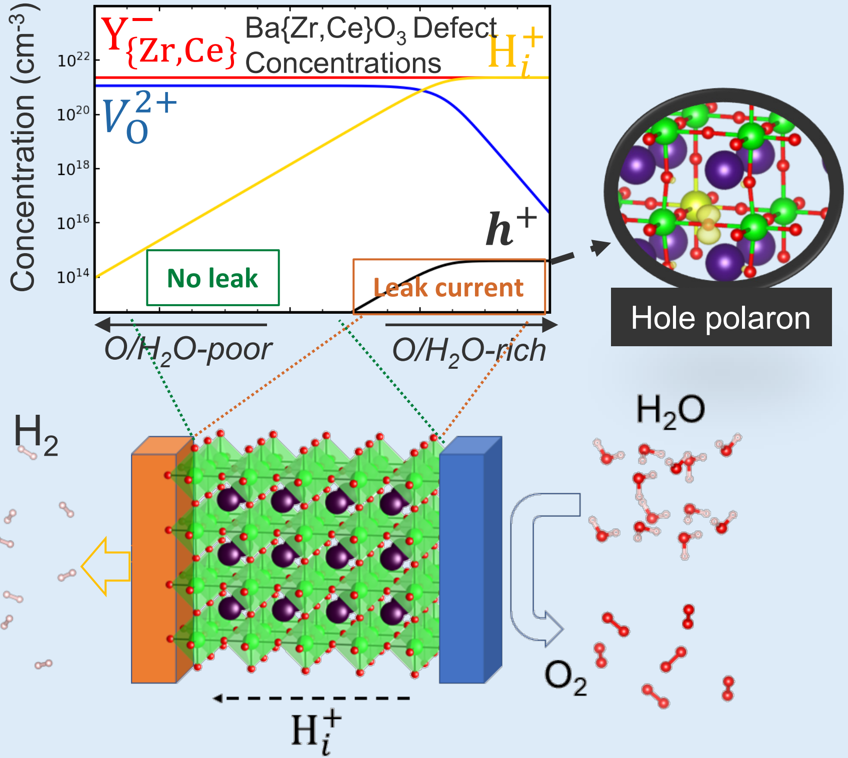


$E_{Ov}$ of 12R-BCM, Mn2-, Mn4-twin

- $E_{12R\text{-}BCM} < E_{Mn4\text{-}twin} < E_{Mn2\text{-}twin}$
- Mn4-twin and Mn2-twin become stable at high-T and low $pO_2$ (at high O vacancy concentration)
- Mn4-twin related to 10H, Mn2-twin related to 6H observed during reduction of 12R-BCM

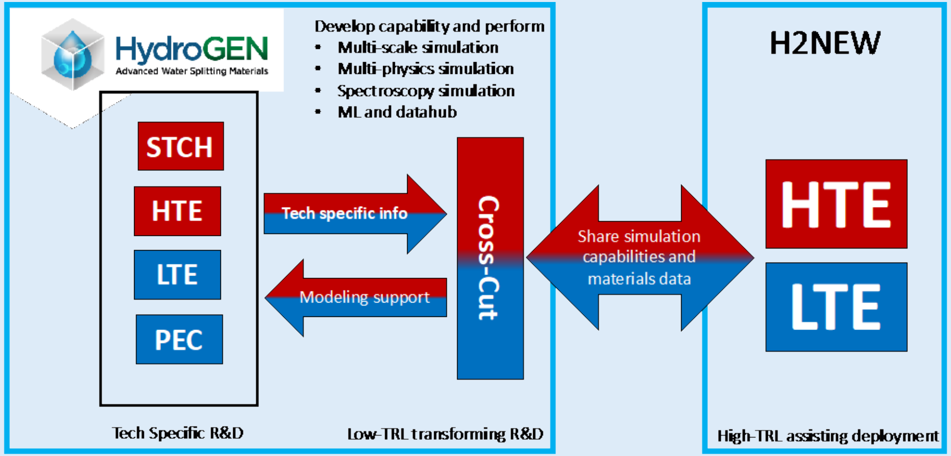
LLNL-SNL. Chem. Mater. 34, 7712 (2023)

## HTE: Polaron formation as leakage mechanism



LLNL-INL. Phys. Rev. Mater. 7, 015402 (2023)

# Cross-Cut Modeling Workshop held on 9/15/2022



- Identify common aspect of computational modeling needed for four technologies
- Share node capabilities between different technologies and maximize effectiveness and efficiencies of modeling support
- Share capabilities, expertise, and knowledge between HydroGEN and H2NEW

Outcome:

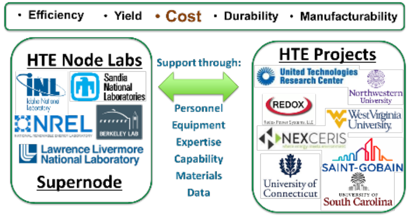
- Low temperature technologies share similar needs in understanding solid-liquid interface under operation condition
- High temperature technologies share many commonalities
  - Thermodynamic analysis of alloy phase diagram including defect analysis
- Modeling effort needs to be complemented by characterization for validation

# Proposed Future Work

- Continue collaborative and integrated research on the five HydroGEN lab R&D projects
    - Achieve the HydroGEN Lab R&D FY23 Annual milestones
- Core labs will execute HydroGEN lab nodes to enable successful phase 3 and new 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
    - Maintain the HydroGEN Data Hub's cyber security compliance
    - Utilize data hub plugins with upgraded infrastructure
    - Streamline user plugins to reduce development efforts on tools not utilized
    - Update user interface to incorporate the H2NEW consortium logo.
- 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)



- Efficiency
- Yield
- **Cost**
- Durability
- Manufacturability

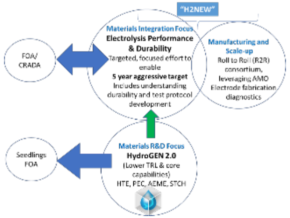
**HTE Node Labs**

**Supernode**

Support through:

Personnel
Equipment
Expertise
Capability
Materials
Data

**HTE Projects**



"H2NEW"

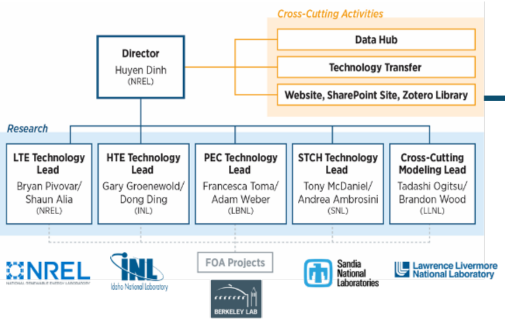
Materials Integration Focus
**Electrolysis Performance & Durability**
Targeted, focused effort to enable
**5 year aggressive target**
Includes understanding durability and test protocol development

Manufacturing and Scale-up
Roll to Roll (R2R) consortium, leveraging AMO
Electrode fabrication diagnostics

FOA/ CRADA

Materials R&D Focus
**HydroGEN 2.0**
(Lower TRL & core capabilities)
HTE, PEC, AEME, STCH

Seedlings FOA



*Cross-Cutting Activities*

**Data Hub**

**Technology Transfer**

**Website, SharePoint Site, Zotero Library**

**Director**
Huyen Dinh
(NREL)

*Research*

| **LTE Technology Lead** | **HTE Technology Lead** | **PEC Technology Lead** | **STCH Technology Lead** | **Cross-Cutting Modeling Lead** |
|---|---|---|---|---|
| Bryan Pivovar/ Shaun Alia (NREL) | Gary Groenewold/ Dong Ding (INL) | Francesca Toma/ Adam Weber (LBNL) | Tony McDaniel/ Andrea Ambrosini (SNL) | Tadashi Ogitsu/ Brandon Wood (LLNL) |

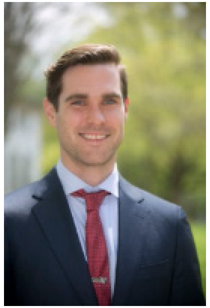
FOA Projects

- 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 Phase 2 annual milestones
  - 5 HydroGEN 2.0 lab projects (AEME, p-SOEC, MS-SOEC, PEC, STCH)
- Continue to connect with H2NEW consortium via cross-cutting modeling and materials development
- Continue to develop technology roadmaps and standard protocols for each AWS technology, publishing protocols, engaging with and disseminating information to the community, and validating protocols
- Continue to develop Data Hub repository, tools, and metadata; Upgrading application infrastructure to maintain security and cyber standards. (https://datahub.h2awsm.org/)
- Continue to connect users to capabilities, publications, research highlights, contacts, and the Data Hub via the HydroGEN website (https://h2awsm.org)

***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***

# Acknowledgements

**This work was fully supported by the U.S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy (EERE), Hydrogen and Fuel Cell Technologies Office (HFTO).**

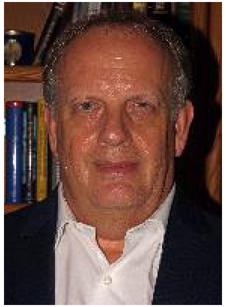

**James Vickers**

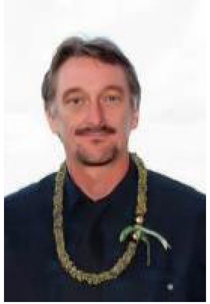

**William Gibbons**


**Rachel Mow**


**David Peterson**


**Katie Randolph**


**Ned Stetson**


**Eric Miller**

# Acknowledgements

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Dan Ginosar
Gabriel Ilevbare
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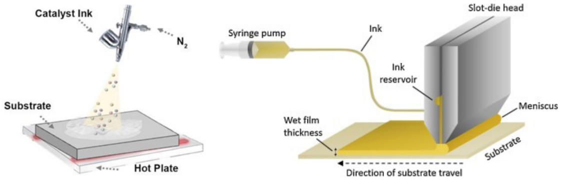
# Technical Backup and Additional Information Slides

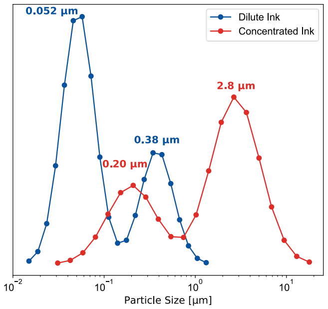
# LTE 2.0 Accomplishments:

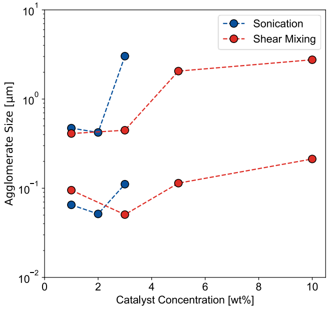
## Ink Characterization and Catalyst Layer Fabrication

- Compared airbrush fabrication (dilute ink, ~1wt% catalyst) to slot die coated electrode (concentrated ink, ~10 wt% catalyst)



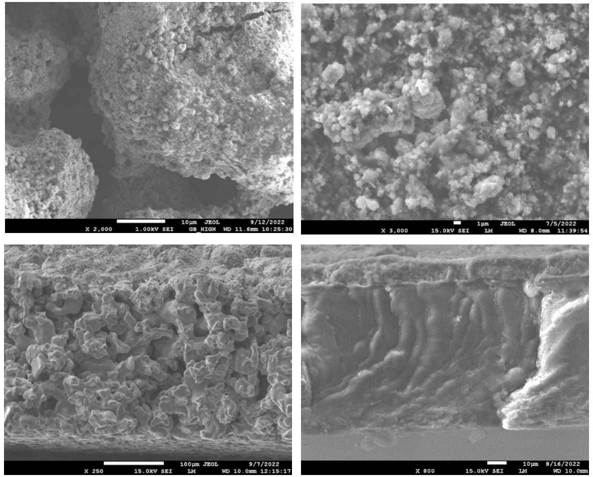
- Increasing ink concentration results in larger catalyst/ionomer agglomerates





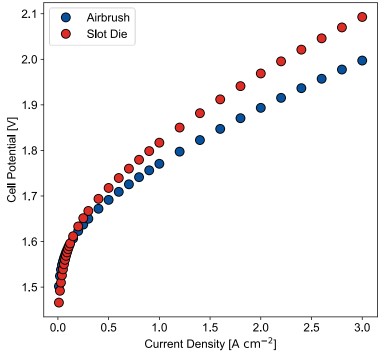
- Larger agglomerates results in larger catalyst particles in the electrode catalyst later

**Airbrush Catalyst Layer** **Slot Die Catalyst Layer**

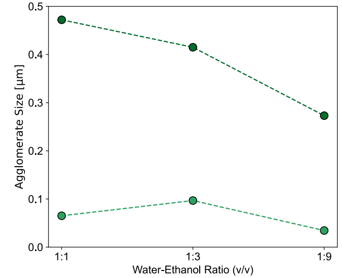


**Airbrush PTE Cross Section** **Slot Die CCM Cross Section**

- Significant discrepancy occurs in cell performance based on fabrication method



- Future work can focus on concentrated ink formulation to control agglomerate size

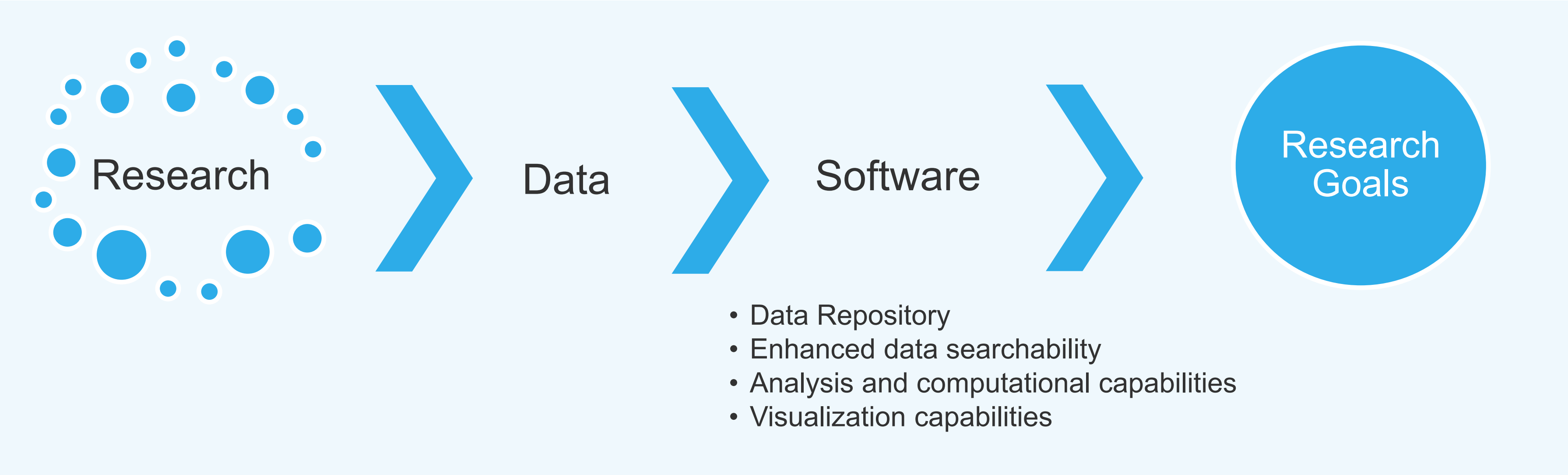


- Catalyst ink concentration influences agglomerate size, catalyst layer properties, and ultimately cell performance
- Controlling ink properties will require tuning of concentrated ink formulations

# Long Term Data Hub Initiative

Improve **Data Searchability** capabilities by expanding searchability and usability of data hubs

1. Retrieve relevant data more easily and quickly
2. Position software to better connect disparate data sources across research consortium
3. Assist future development of machine learning algorithms and predictive capabilities



- Data Repository
- Enhanced data searchability
- Analysis and computational capabilities
- Visualization capabilities

# Technology Transfer Activities

- HydroGEN EMN has developed four standard, pre-approved technology transfer agreements between all consortium partners to enable streamlined access:
  - Non-Disclosure Agreement (NDA)
  - Intellectual Property Management Plan (IPMP)
  - Materials Transfer Agreement (MTA)
  - Cooperative Research and Development Agreement (CRADA)
- HydroGEN has executed 33 project NDAs and 2 MTAs
- Tech transfer in HydroGEN occurs organically via collaboration between lab capability nodes and industry partners in the different AWS technologies
- Continue to develop IP and follow the IPMP developed by the HydroGEN consortium
- Patent Applications:
  - T. He, D. Ding, W. Wu. Methods and systems for hydrogen gas production through water electrolysis, and related electrolysis cells. US Patent (16/483,631), Granted, 2021.
  - D. Ding, W. Bian, W. Wu. Facile methods to rejuvenate electrolyte surface for high-performing protonic ceramic electrochemical cells. US Patent Provisional Application (63/298,084), 2022.
  - A. Mohite, M. Wong, A. Fehr, A. Agrawal, F. Mandani, Conductive Adhesive-Barrier Enabling Integrated Photoelectrodes for Solar Fuels. Provisional Application for U.S. Letters Patent (22511 Patent Trademark Office).

# Special Recognitions and Awards

- Huyen Dinh: NREL’s Foundation Outstanding Woman in STEM
- Two innovative technologies with ties to the HydroGEN Advanced Water Splitting Materials consortium have been honored with a 2022 R&D 100 Award from R&D World magazine
  - **PGM-Free OER Catalyst as Replacement of Iridium for PEM Water Electrolyzer**
    - Technology was developed through a HydroGEN seedling project led by Di-Jia Liu, ANL
  - **Solar Fuel Generator Including a Catalytic Mesh**
    - Inventors include current and former HydroGEN capability experts Jeff Beeman, Frances Houle, and David Larson from LBNL, and knowledge gained through the device development has led to other HydroGEN achievements, including a scaled-up integrated photoelectrochemical device demonstration published in 2020.

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8. Shen, X.; Yanagi, R.; Solanki, D.; Su, H.; Li, Z.; Xiang, C.-X.; Hu, S. Comprehensive Evaluation for Protective Coatings: Optical, Electrical, Photoelectrochemical, and Spectroscopic Characterizations. *Frontiers in Energy Research* **2022**, *9*. https://doi.org/10.3389/fenrg.2021.799776.
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# Publications, cont.

15. R. T. Bell†, N. A. Strange†, D. A. Plattenberger, S. Shulda, J. E. Park, A. Ambrosini, K. N. Heinselman, J. D. Sugar, P. A. Parilla, E. N. Coker, A. McDaniel, D. Ginley, "Synthesis of High-Purity BaCe0.25Mn0.75O3; an Improved Material for Thermochemical Water Splitting," *Acta. Crystallogr. B.* 2022-12-01, 78, 6, 884-892. 10.1107/S2052520622010393
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# Publications, cont. (submitted, accepted, under review, in press)

32. E.K. Volk, S. Kwon, S.M. Alia, “Catalytic activity and stability of non-platinum group metal oxides for the oxygen evolution reaction in anion exchange membrane electrolyzers,” Journal of the Electrochemical Society (2023) [Under Review]
33. Todd G. Deutsch, “Concentrating on solar for hydrogen”, Nature Energy, April, 2023. Accepted manuscript. DOI : 10.1038/s41560-023-01256-1.
34. Z. Song, C. Li, L. Chen, K. Dolia, S. Fu,N. Sun, Y. Li, K. Wyatt, J. Young, T. Deutsch, Y. Yan, “All-perovskite tandem photoelectrodes for unassisted solar hydrogen production.” ACS Energy Letters (under review).
35. Y. Xiao, X. Kong, S. Vanka, W. J. Dong, G. Zeng, Z. Ye, K. Sun, I. A. Navid, B. Zhou, F. M. Toma, H. Guo, Z. Mi, "Oxynitrides enabled photoelectrochemical water splitting with over 3,000 hrs stable operation in practical two-electrode configuration", Nature Communication 2023, accepted
36. Z. Song, C. Li, L. Chen, K. Dolia, S. Fu, N. Sun, K. Wyatt, J. Young, T. Deutsch, Y. Yan. "All-perovskite tandem photoelectrodes for unassisted solar hydrogen production.” Under review at ACS Energy Letters.
37. A. M.K. Fehr, A. Agrawal, F. Mandani, C. L. Conrad, Q. Jiang, S. Y. Park, O. Alley, B. Li, S. Sidhik, I. Metcalf, C. Botello, J. Young, J. Even, J. C. Blancon, T. G. Deutsch, K. Zhu, S. Albrecht, F. M. Toma, M. Wong and A. D. Mohite, "Integrated halide perovskite photoelectrochemical cells with solar-driven water-splitting efficiency of 20.8%,” submitted.
38. M.M. Welander, B. Hu, M.C. Tucker, "Optimization of metal-supported solid oxide electrolysis cells with infiltrated catalysts," *Int. J. Hydrogen Energy*, in press

# Presentations

1. E.K. Volk, “Establishing half- and single- cell baselines for the oxygen evolution reaction (OER) on non- platinum group metal (PGM) oxide electrocatalysts in alkaline media”, Poster Presentation, International Conference on Electrolysis, (July 2022)
2. E.K. Volk, “Establishing half- and single- cell baselines for the oxygen evolution reaction (OER) on non- platinum group metal (PGM) oxide electrocatalysts in alkaline media”, Oral Presentation, ACS Colloids and Surface Science Symposium, (July 2022)
3. X. Peng, “The Cutting-edge in Clean Electrolysis for Green Hydrogen Production”, Invited talk, U.S. Frontiers of Engineering Symposium (September 22, 2022)
4. X. Peng, “Pathways to Terawatt Scale Electrolysis____ Importance of Interfaces and Underexplored Opportunities”, Fuel Cell Gordon Research Conference (July 27, 2022)
5. A. W. Tricker, “Tuning Catalyst-Ink Formulations for Blade Coating of Hydroxide-Exchange-Membrane Water Electrolyzers”, 242nd ECS meeting (October 9-13,2022)
6. X. Peng, “The Cutting-edge in Clean Electrolysis for Green Hydrogen Production”, Invited talk, U.S. Frontiers of Engineering Symposium (September 22, 2022)
7. X. Peng, “Pathways to Terawatt Scale Electrolysis____ Importance of Interfaces and Underexplored Opportunities”, Fuel Cell Gordon Research Conference (July 27, 2022)
8. A. W. Tricker, “Tuning Catalyst-Ink Formulations for Blade Coating of Hydroxide-Exchange-Membrane Water Electrolyzers”, 242nd ECS meeting (October 9-13,2022)
9. F. Toma , “Photoelectrochemical Fuel Generation: Light Absorbers Under the Spotlight”, invited talk, Renewable Energy: Solar Fuels (Gordon Research Conference), Italy. May 8-13, 2022. Invited talk.
10. T. Deutsch, “III-V’s via Hydride Vapor Phase Epitaxy for Photoelectrochemical Water Splitting” 2022 Spring Meeting and Exhibit of the Materials Research Society, Honolulu, HI. May 12, 2022. Contributed Talk

# Presentations, cont.

11. T. Deutsch, “Fundamentals and Current State of Photoelectrochemical Water Splitting” Technical University of Denmark Surfcat Summer School, Kysthusene, Denmark. August 8, 2022. Invited Talk
12. F. Toma, “Design and characterization of integrated systems for solar fuel production” UC Davis Energy and Efficiency Institute Seminar, California. Sept. 30th, 2022. Invited lecture.
13. Y. Yan, “All perovskite tandem photoelectrodes for efficient unassisted water splitting,” 242nd ECS meeting, Atlanta, GA. 10/9/2022. Invited talk.
14. F. Toma, “All perovskite tandem photoelectrodes for efficient unassisted water splitting,” 242nd ECS meeting, Atlanta, GA . 10/9/2022. Invited talk
15. T. Deutsch, “III-V Semiconductors for Photo-Electrochemical Hydrogen Production: Recent Progress in Efficiency, Durability, and Cost” Southeastern Regional Meeting of the American Chemical Society, San Juan, PR. October 20, 2022. Invited talk.
16. T. Deutsch, “Photo-Electrochemical Water Splitting for Solar Hydrogen Fuel Production” University of New Hampshire Lab Day, UNH, Durham, NH. October 27, 2022. Invited Talk.
17. F. Toma Invited talk, “Design and characterization of integrated systems for solar fuel production”, SERMACS 2022, The Chemistry of Solar Fuels Symposium, Puerto Rico. October 19-22, 2022. Invited talk.
18. M. Steiner, “Photovoltaics beyond just terrestrial solar: Applications for energy storage, solar fuels and more,” Massachusetts Institute of Technology Department of Mechanical Engineering seminar. November 4, 2022. Invited Talk
19. T. Deutsch, “Photo-Electrochemical Water Splitting for Solar Hydrogen Fuel Production” Student Chapter of the Electrochemical Society Seminar (virtual), Notre Dame University. January 25, 2023. Invited Talk
20. A. M.K. Fehr, A. Agrawal, F. Mandani, O. Alley, B. Li, S. Albrecht, F.M. Toma, M.S. Wong, A. D. Mohit, “Integrated Photoelectrochemical Devices for Solar Water-Splitting with Silicon-Perovskite Tandems at >21% STH,” Presentation at MRS Spring Meeting, April 2023

# Presentations, cont.

21. K. Huang, “Developing Barrier Layer Free Oxygen Electrode for Solid Oxide Cells”, ECS241, invited talk, May 29-June 2, 2022, Vancouver, Canada.
22. K. Huang, “Exploring the Safe Operational Boundary for High-Temperature Solid Oxide Electrolyzer”, invited talk, ECS241, Vancouver, May 29-June 2, 2022, Vancouver, Canada.
23. K. Huang, “SOC research activities at USC”, June 4, 2022, PNNL, WA.
24. P. Jayaprakasam, Y. Wen, K. Huang, X. Jin, "Understanding Delamination of Oxygen Electrode by Electro-Chemical and Mechanical Coupled Modeling," 23rd International Conference on Solid State Ionics, Boston, MA, 07/21/2022
25. P. Jayaprakasam, Y. Wen, K. Huang, X. Jin, "Electro-Chemo-Mechanical Coupled Modeling of Oxygen Electrodes in Solid Oxide Electrolyzer Cells," 241st ECS Meeting, Vancouver, Canada, 05/29/2022-06/02/2022
26. K. Cook, J. Wrubel, Z. Ma, K. Huang, P. Jayapragasam, and X. Jin, "Modeling Electrokinetics of Oxygen Electrodes in Solid Oxide Electrolyzer Cells," 241st ECS Meeting, Vancouver, Canada, 05/29/2022-06/02/2022
27. M.C. Tucker, F. Shen, M.M. Welander, B. Hu, "Metal-supported solid oxide electrolysis cells," *International Conference on Electrolysis*, 2022, Golden, CO
28. M.C. Tucker, B. Hu, M.M. Welander, F. Shen, G.Y. Lau, "Metal-Supported Solid Oxide Cells for Chemical Conversion, Electrolysis, and Power Production," *Eur. Fuel Cell Forum*, 2022, Lucerne, Switzerland
29. M.C. Tucker, F. Shen, M.M. Welander, "Metal-supported solid oxide electrolysis cells with coatings to suppress chromium migration," *242nd ECS Meeting*, 2022, Atlanta, GA
30. M.C. Tucker, F. Shen, M.M. Welander, B. Hu, Z. Zhu, "Metal-supported Solid Oxide Fuel Cells and Electrolyzers for Low-cost, Robust, Rapid-start Systems," *Hydrogen and Fuel Cell Seminar*, 2022, Long Beach, CA

# Presentations, cont.

31. T. Ogitsu, “Computational Modeling of Photoelectrochemical Processes for Hydrogen Production,” 242th ECS, Atlanta GA. 2022. Invited.
32. T. Ogitsu, “Ab initio studies of elemental processes in water splitting technologies,” 7th Conference on Catalysis and Chemical Engineering, Las Vegas, NV, Feb 2023. Invited.
33. B.C. Wood, “Multiscale materials modeling for hydrogen production.” Invited.
34. S. Intikhab, E.K. Volk, R.R. Beswick, H. Yu, D.A. Cullen, S. Kwon, S.M. Alia, “Materials Integration, Catalyst-Ionomer Interfaces, and Durability Implications in Anion Exchange Membrane-Based Low Temperature Electrolysis” 243rd ECS Meeting (May 28 – June 2, 2023)
35. E.K. Volk, R.R. Beswick, S. Kwon, S.M. Alia, “Electrochemical Activation of NiFe2O4 for the Oxygen Evolution Reaction in Alkaline Media” 243rd ECS Meeting (May 28 – June 2, 2023)
36. S.M. Alia, S. Intikhab, M.-A. Ha, S. Ghosal, “(*Invited*) Materials Integration, Durability, and Perspectives in Anion Exchange Membrane-Based Low Temperature Electrolysis” 241st ECS meeting (May 29 – June 2, 2022)
37. A. W. Tricker, “Tuning Catalyst-Ink Formulations for Blade Coating of Hydroxide-Exchange-Membrane Water Electrolyzers”, 242nd ECS meeting (October 9-13,2022)

# Presentations, cont.

38. H.N. Dinh, “Hydrogen Production and Hydrogen Shot: Options for Producing Low-Carbon Hydrogen at Scale,” Presented at the MIT Energy Initiative Spring Symposium May 10, 2022. https://www.nrel.gov/docs/fy22osti/82933.pdf (invited)
39. H.N. Dinh, S. Alia, B. Pivovar, F. Toma, A. Weber, D. Ding, G. Groenewold, A. McDaniel, A. Ambrosini, T. Ogitsu, and B. Wood, “HydroGEN Overview: A Consortium on Advanced Water Splitting Materials,” Oral presentation P148 at the DOE Hydrogen Program 2022 Annual Merit Review and Peer Evaluation Meeting, June 2022. https://www.nrel.gov/docs/fy22osti/83179.pdf
40. H.N. Dinh, “Hydrogen Energy Earthshot and NREL’s Role” 2022 ECS Canada Section Spring Meeting, University of Calgary, CANADA, June 12, 2022, (Invited)
41. H.N. Dinh, “Technologies for a Hydrogen Economy”, Invited Discussion Leader for the 2022 Fuel Cell Gordon Research Conference, Bryant University, Smithfield, RI, July 27, 2022.
42. H.N. Dinh, “Clean Hydrogen Production R&D at NREL”, FECM Research Experience in Carbon Sequestration (RECS) Workshop http://recs-ccus.org/ – invited talk, NREL, Sept. 13, 2022.
43. H.N. Dinh, “HydroGEN Advanced Water Splitting Materials Capabilities Overview” oral presentation, HFTO’s monthly H2IQ Webinar, virtual, Sept. 16, 2022. H2IQ Hour: HydroGEN Advanced Water Splitting Materials Capabilities Overview | Department of Energy
44. H.N. Dinh, “Hydrogen is an important sector coupling”, virtual oral presentation and panel member, IRENA Coalition for Action, Sector Coupling: a key concept for accelerating the energy transition, Dec. 12, 2022. (Invited)
45. H.N. Dinh, “Clean hydrogen: energy carrier, renewables enabler, and sector coupler to accelerate the energy transition and meet climate goals”, RE3 Workshop: Clean Hydrogen and Industrial Decarbonization, Louisville, Kentucky, Mar. 9, 2023. (Invited).
46. H.N. Dinh, Emily Harrell, Christina Vader, Rachel Hurst, “HydroGEN and H2NEW Data Hub”, H2NEW Consortium In-Person Meeting, Napa, CA Mar. 14, 2023.

# FY2023 Q1 Milestones

| Quarter/ Type | Due Date | Status | Milestone Name/Description |
|---|---|---|---|
| Q1<br>Progress measure | 12/31/22 | Complete | **PEC photoreactor cell design (NREL)**: Submit design for hand-held PEC photoreactor cell for fabrication or 3D printing. **Criteria:** The cell should minimize electrode separation distance, accommodate 4cm$^2$ of absorber, look good, and be leak free. (NREL, LBNL) |
| Q1<br>Progress measure | 12/31/22 | Complete | **STCH Materials Assessment : (SNL)** Select FeAl2O4 and CeO2 as initial exemplar materials. Where necessary, synthesize materials and map delta-T-pO2 state space over specific cycle conditions using validated TGA and flow reactor protocols. Apply a material evaluation formalism that projects material thermodynamic and kinetic information onto a radar chart containing a minimum of 4 axes (normalized to CeO2). Axes as follows: 1) mole O2/mole oxide atoms measured in reduction, 2) mole H2/mole oxide atoms measured in steam oxidation, 3) ∆G0(298K, water thermolysis) / ∆H0 (reduction) which is the maximum possible theoretical efficiency, and 4) time required to achieve 90% of H2 produced (i.e., ∆delta) under specific cycle conditions. (NREL, SNL). |
| Q1<br>Progress measure | 12/31/22 | Complete | **Integration of Models Across Technologies (LLNL):** Devise plan to integrate one of the primary multiscale modeling frameworks (electrochemical kinetics, mass transport, or phase transformation kinetics) to at least two water-splitting technologies to demonstrate its crosscutting nature |

# FY2023 Q2 Milestones

| Quarter/ Type | Due Date | Status | Milestone Name/Description |
|---|---|---|---|
| Q2<br>Progress measure | 3/31/23 | On Track | **STCH material synthesis (NREL-Bell):** Synthesize 3 of the computationally predicted stoichiometries for new STCH materials derived from efforts of NREL, LLNL & Sandia and perform preliminary thermal stability assessment and by quantifying the phase fraction of the desired phases using quantitative synchrotron X-ray diffraction analysis before and after thermal aging. **Criteria:** Perform initial investigations into these and related SNL materials by carrying out preliminary thermal stability assessment primarily by TGA/DSC-RGA cycling and through using lab and synchrotron-based techniques to quantify the phase fraction and impurity phase formation using quantitative synchrotron X-ray diffraction analysis before and after thermal aging. As warranted, use advanced techniques to confirm oxidation states and site occupancies in cycled materials. (NREL, LLNL, SNL) |
| Q2<br>Progress measure | 3/31/23 | On Track | **STCH Machine Learning Modeling (SNL):** Complete second round of DFT calculations to support ML model. Make DFT defect data available in datahub. Use ML model to screen for STCH materials with desired defect enthalpy using NRELmatDB and Materials Project structures based on new second round elements. Define next steps to increase ML model complexity and enhance materials discovery capability (i.e., add charged defects). (NREL, SNL) |
| Q2<br>Progress measure | 3/31/23 | On Track | **Cross-Cutting Modeling: PEC Durability (LLNL):** Demonstrate strategy to model surface structure and stability of III-V photoelectrodes by integrating atomistic and spectroscopic simulations with characterization. Work with LBNL to establish foundational understanding of materials degradation. |

# FY2023 Q3 Milestones

| Quarter/ Type | Due Date | Status | Milestone Name/Description |
|---|---|---|---|
| Q3<br>Progress measure | 6/30/23 | **On Track** | **Extension of the current machine learning (ML) model for STCH material defect energies (NREL-Lany):** We will execute a second set of high-throughput DFT calculations that will allow us to train the ML model for approximately double the number of cationic elements that have the potential do STCH water splitting. **Criteria:** Using this extended ML model, we will screen at least 4 times as many oxides (compared to the current model) in existing databases for their potential performance in STCH. |
| Q3<br>Progress measure | 6/30/23 | **On Track** | **STCH Model Improvement (LLNL):** Demonstrate strategy to incorporate entropy, anharmonicity, and/or defects to improve fidelity of STCH material thermodynamics computation. Work with SNL and NREL to incorporate into machine learning models for material selection. |
| Q3<br>Progress measure | 6/30/23 | **On Track** | **Cross-Cutting Modeling (SNL):** Model the relative stability of competing phases under STCH relevant redox cycle conditions, as well as how gas partial pressure of H2 and O2 impact phase evolution. Coordinate lab efforts to leverage ML techniques for accelerating STCH materials development. (LLNL, NREL, SNL). |

# FY2023 Q4 Milestones

| Quarter/ Type | Due Date | Status | Milestone Name/Description |
|---|---|---|---|
| Q4<br>Annual Milestone | 9/30/23 | On Track | **LTE AEM:** Incorporating experiment and modeling, down-select AEM supporting electrolytes (type, concentration) and operating conditions (materials choices, flow configurations, temperature) that demonstrate cell overvoltage within 50 mV (HFR-free) of commercial Nafion at 1 A/cm2 (NREL, LBNL, SNL). **Criteria:** Demonstrate AEMWE in a supporting electrolyte with a cell overvoltage within 50 mV (HFR-free) of commercial Nafion at 1 A/cm2. |
| Q4<br>Annual Milestone | 9/30/23 | On Track | **LTE AEM (SNL): Provide Microscopy Data to Support AEM down-select:** SEM and TEM imaging and compositional analysis of electrodes to understand aging and degradation processes by quantifying the extent of catalysts redistribution, dispersion, and deactivation; revealing changes in catalyst layer thickness, porosity, pore size distribution, particle size, etc., that lead to ohmic losses. |

# FY2023 Q4 Milestones

| Quarter/ Type | Due Date | Status | Milestone Name/Description |
|---|---|---|---|
| Q4<br>Annual Milestone | 9/30/23 | On Track | **PEC (NREL):** Demonstrate a completely integrated system and neutral pH conditions that achieve >220 h durability at short circuit and > 5% STH efficiency. Scale-up to a hand-held >4 cm2 active area device that will split water under direct sunlight illumination with appreciable hydrogen bubble generation. **Criteria:** Demonstrate a completely integrated system and neutral pH conditions that achieve >220 h durability at short circuit and > 5% STH efficiency. Scale-up to a hand-held >4 cm2 active area device that will split water under direct sunlight illumination with appreciable hydrogen bubble generation. |
| Q4<br>Progress measure | 9/30/23 | On Track | **PEC (LBNL):** For short-circuit demonstrations in neutral pH at STH > 10%, a photocathode has operated for 200 h in pH 7 without a membrane separator and a photoanode for 110 h in pH 9.3 with a bipolar membrane. **Criteria:** Demonstrate a complete device assembly and neutral pH conditions that achieve >220 h durability at short circuit and > 5% STH efficiency. Scale-up to a hand- held > 4 cm2 active area device that will split water under direct sunlight illumination with appreciation bubble generation. (LBNL, NREL) |
| Q4<br>Annual Milestone | 9/30/23 | On Track | **MS-SOEC cell structure, composition, and processing established (LBNL):** Gen 4 cell operated for >500 h at constant inlet steam content of 50% or higher, current density (chosen to give initial voltage around 1.3 to 1.4 V), and temperature around 700°C. Final target is: >1A/cm2 at 1.4V, 700°C, 50:50 H2O:H2; <5%/kh degradation at 0.5 A/cm2. |
| Q4<br>Annual Milestone | 9/30/23 | On Track | **p-SOEC electrolyte R&D (INL):** Develop a robust, energy-efficient, and reliable electrolyte, for p-SOEC at 500-600°C, that has proton conductivity > 0.02 S cm-2 at 600°C, by understanding the proton conduction and electronic leakage mechanisms. Achieve > 95% Faradaic efficiency when steam concentration is > 50% at 600°C or lower (> 1 A cm$^{-2}$ at 1.3 V), tested for a minimum of 500 hours. |

# FY2023 Q4 Milestones

| Quarter/ Type | Due Date | Status | Milestone Name/Description |
|---|---|---|---|
| Q4<br>Progress measure | 9/30/23 | On Track | **Conduct STCH Material Down-select (SNL):** Use the technology assessment methodology derived during the course of this project, and baselined or "calibrated" against the CeO2 cycle, to evaluate material viability. The metric accounts for material-specific cycle dynamics and plant operational modality. A selected group of known and new materials (i.e., best materials produced by HydroGEN seedling projects) will be evaluated for their potential to meet DOE STCH technology performance targets (~6 materials including ceria). (lead SNL, NREL, LLNL) |
| Q4<br>Annual Milestone | 9/30/23 | On Track | **Demonstration of Crosscutting Models for Electrochemical Kinetics (LLNL):** Successfully demonstrate crosscutting modeling capability for multiscale electrochemical kinetics by applying to IrO2 PEC systems with varying surface orientations under at least two operating modes. Show ability of the model to reproduce experimental trends within 70%. |
| Q4<br>Annual Milestone | 9/30/23 | On Track | **Demonstration of Crosscutting Models for Ion Transport Kinetics (LLNL):** Successfully demonstrate crosscutting modeling capability for multiscale ion transport kinetics by applying to at least three different proton-conducting HTE electrolyte formulations. Show ability of model to correctly reproduce experimental trend across either grain size or composition. |

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