Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

Hydrogen Consortium: Technical Progress on Renewable Hydrogen Production R&D

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

Date: October 10, 2023

244th ECS Meeting, Gothenburg, Sweden

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

What is the Hydrogen Energy Earthshot goal?

ENERGY earthshots U.S. DEPARTMENT OF ENERGY | Hydrogen

Hydrogen Energy Earthshot

"Hydrogen Shot"

"1 1 1"
$1 for 1 kg clean hydrogen in 1 decade

Launched June 7, 2021
Summit Aug 31-Sept 1, 2021

S. Satyapal, et al., "Overview of DOE RFI Supporting Hydrogen Bipartisan Infrastructure Law Provisions, Environmental Justice, and Workforce Priorities, Feb. 24, 2022

DEPARTMENT OF ENERGY UNITED STATES OF AMERICA

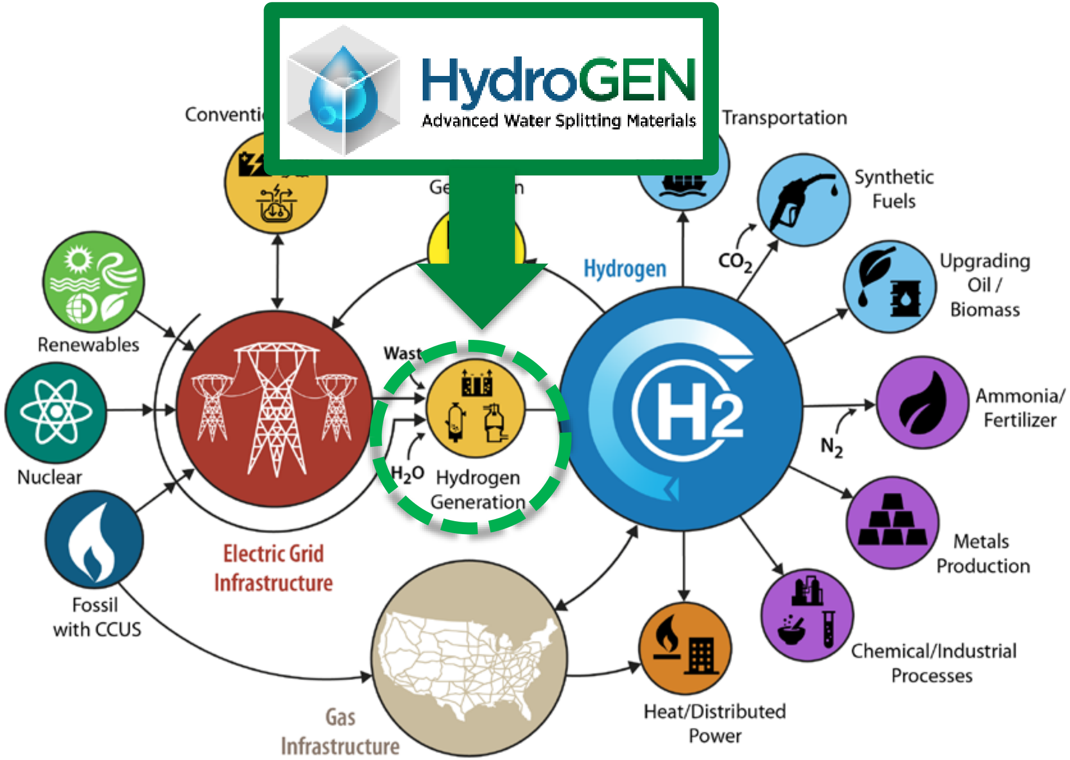
Bipartisan Infrastructure Law – Hydrogen Highlights

- **Covers $9.5B** for clean hydrogen:
  - $8B for at least 6-10 regional clean H_2 hubs
  - $1B for electrolysis RD&D
  - $0.5B for clean H_2 technology manufacturing and recycling R&D
- Aligns with Hydrogen Shot priorities by directing work to reduce the cost of clean hydrogen to $2 per kilogram by 2026
- Requires developing a National Hydrogen Strategy and Roadmap

President Biden Signs the Bipartisan Infrastructure Bill into law on November 15, 2021. Photo Credit: Kenny Holston/Getty Images

S. Satyapal, et al., "Overview of DOE RFI Supporting Hydrogen Bipartisan Infrastructure Law Provisions, Environmental Justice, and Workforce Priorities, Feb. 24, 2022

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



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

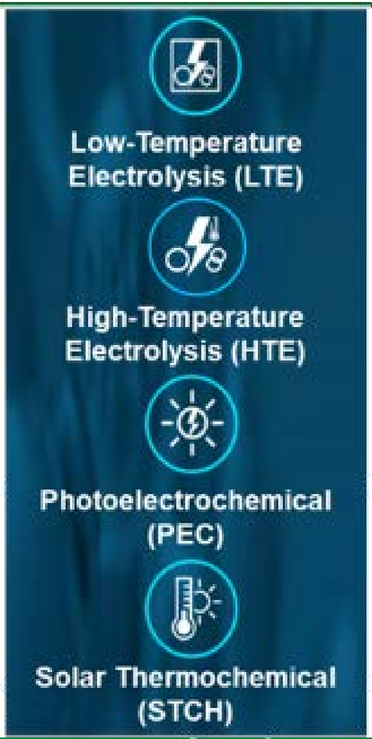
"Hydrogen at Scale (H_2@Scale): Key to a Clean, Economic, and Sustainable Energy System," Bryan Pivovar, Neha Rustagi, Sunita Satyapal, *Electrochem. Soc. Interface* Spring 2018 27(1): 47-52; doi:10.1149/2.F04181if.

HydroGEN Consortium

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

Goal: Accelerating R&D of innovative advance water splitting (AWS) materials and technologies for clean, sustainable and low-cost hydrogen production.

Water



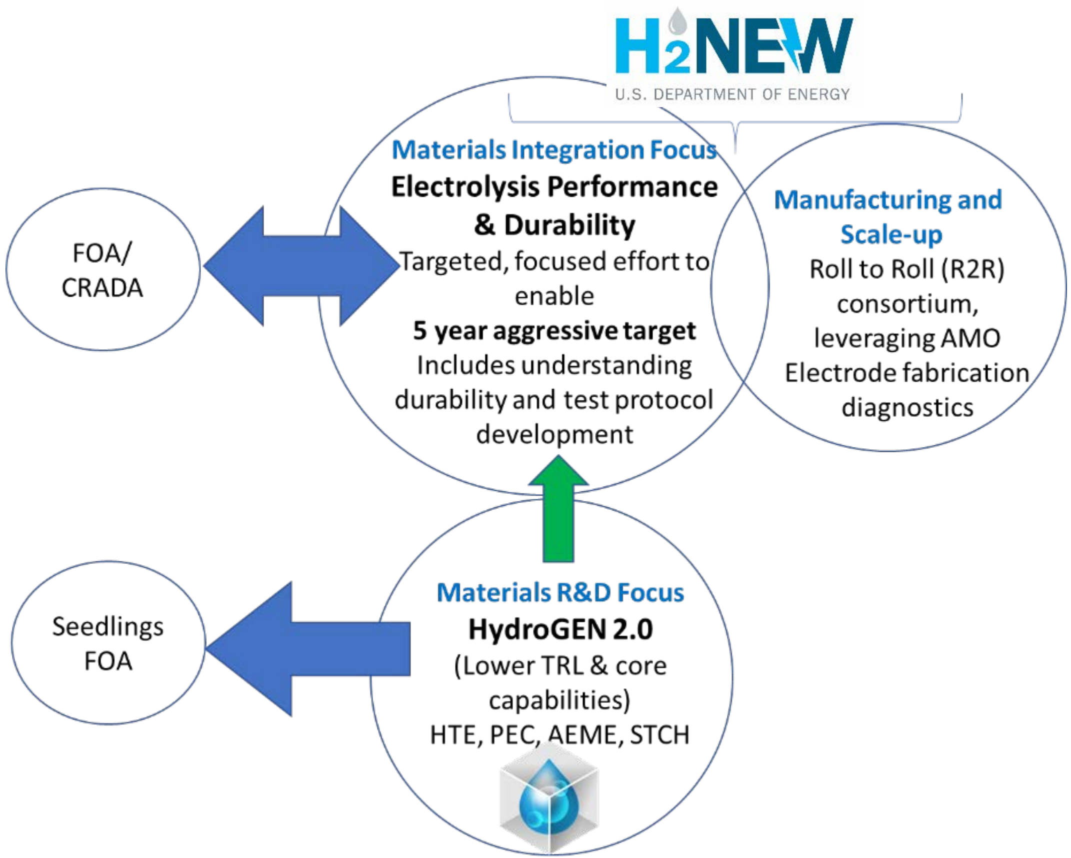
National Lab Consortium Team

- NREL – National Renewable Energy Laboratory
- Berkeley Lab
- INL – Idaho National Laboratory
- Sandia National Laboratories
- Lawrence Livermore National Laboratory

H_2 Production Target: $1/kg

HydroGEN is advancing Hydrogen Shot goals by fostering 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

HydroGEN Materials R&D Feeds to H2NEW Materials Integration



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)

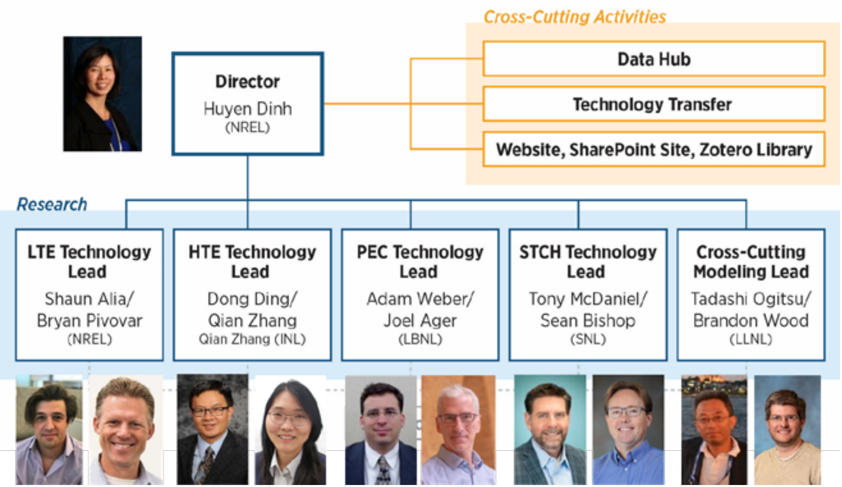
Solar thermochemical (STCH)

HydroGEN Lab R&D + Lab Capability Support

EMN Collaboration and Approaches

HydroGEN 2.0: Lab R&D

Early-Stage Materials R&D Projects



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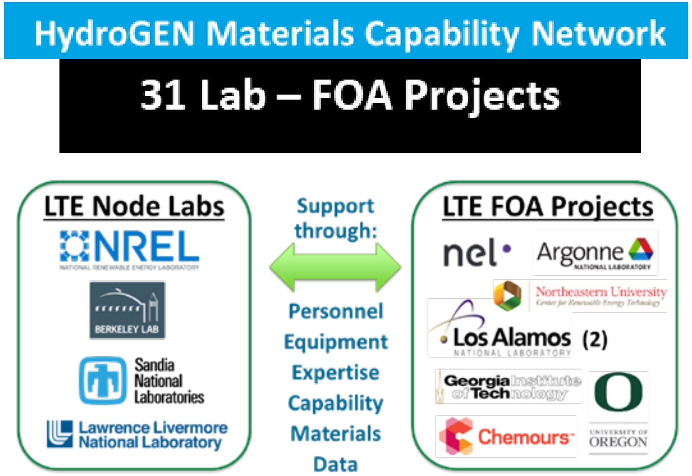
HydroGEN 1.0: Lab Support

Lab capabilities + experts support projects



11 New PEC and STCH Projects Awarded

New PEC Projects

1. Rice University, **Aditya Mohite**
2. University of Toledo, **Yanfa Yan**
3. University of Michigan, **Zetian Mi**
4. University of Hawaii Manoa, **Nico Gaillard**
5. California Institute of Technology, **Joel Haber**
6. Yale University, **Shu Hu**

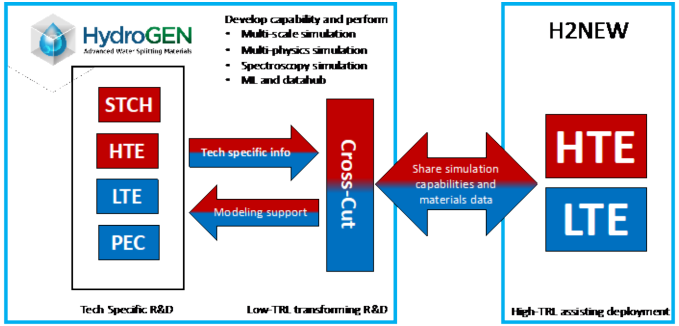
New STCH Projects

1. University of Colorado Boulder, **Al Weimer**
2. Arizona State University, **Chris Muhich**
3. Washington University in St. Louis, **Robert Wexler**
4. University of Colorado Boulder, **Charles Musgrave**
5. Saint-Gobain, **Xin Qian**

Science Challenges for HydroGEN 2.0 Lab R&D

- ***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



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I01F-2070, Shaun Alia

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

I06-2409, Anh T. Pham

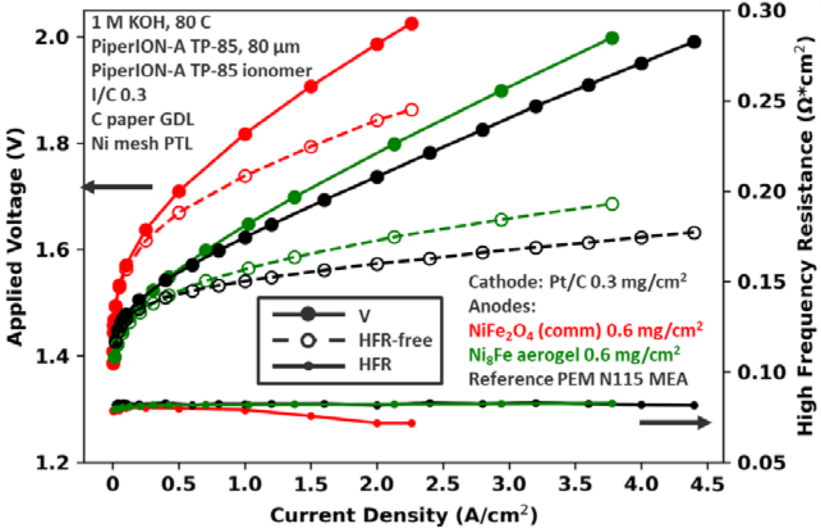
I06-2419, Dong Ding

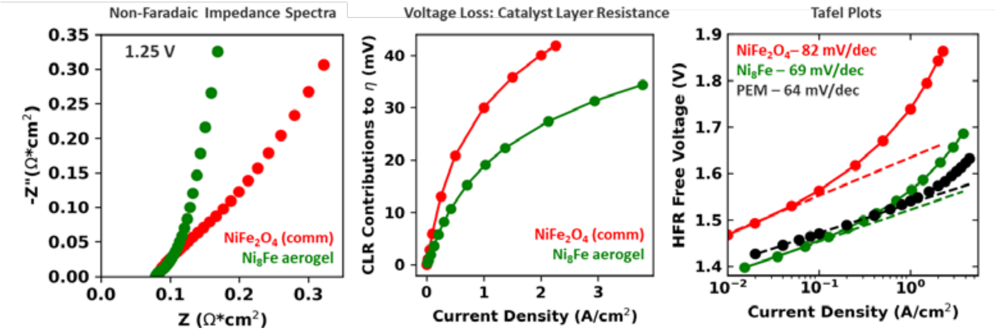
I05-2349, Todd Deutsch

I06-2420, Sean Bishop

Progress Towards LTE Performance Milestone of PGM-free OER Catalyst

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/cm^2. 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).*





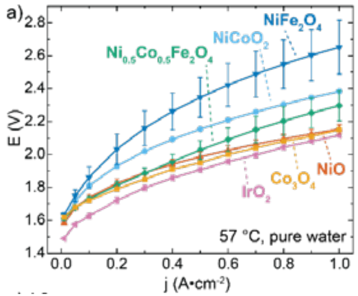
System	HFR (Ω cm^2)	CLR (Ω cm^2)	Tafel (mV/dec)	$V_{HFR\text{-}free}$ (V) at 1.0 A cm^{-2}
$NiFe_2O_4$	0.078	0.197	82	**1.739**
NiFe 8:1	0.082	0.078	69	**1.559**
PEM 115 MEA	0.083	0.008	64	**1.541**

- **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/cm^2".* (*HFR*-free voltage for NiFe 8:1 catalyst is within 18 mV of the PEM 115 MEA performance.)

HydroGEN LTE Seedling Projects with Lab Capability Support

- **(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.

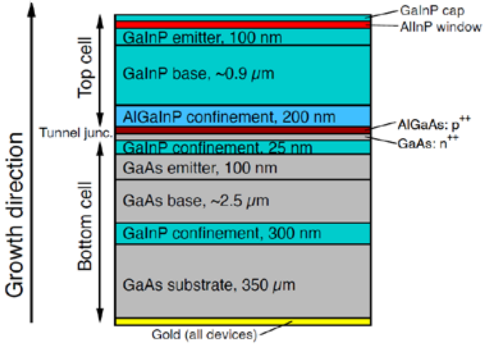
- **(UO and NREL, LBNL, SNL) Pure Hydrogen Production through Precious-Metal-Free Membrane Electrolysis of Dirty Water:** Identified and characterized key degradation modes of AEM electrolysis in pure and contaminated water associated with ionomer oxidation at the anode and develop new catalyst and mitigation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



HydroGEN PEC Lab R&D Technical Progress

Photoelectrode growth by metal organic vapor phase epitaxy (MOVPE)

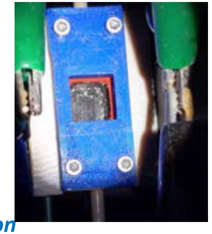
MOVPE at 620℃ growth temperature



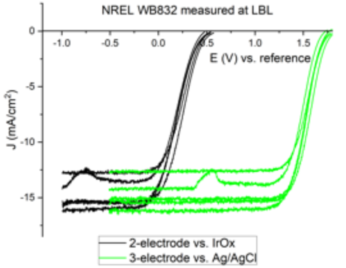
Schematic of the III-V high efficiency photoelectrode

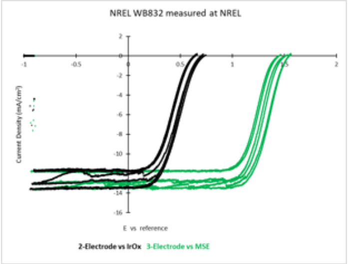
Photoelectrode Fabrication and Testing at NREL and LBNL

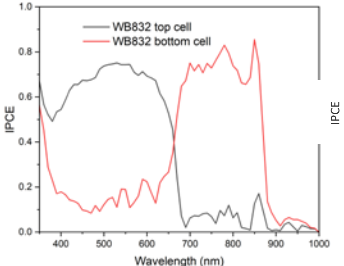
Dual anode cell with high modularity and ease of fabrication

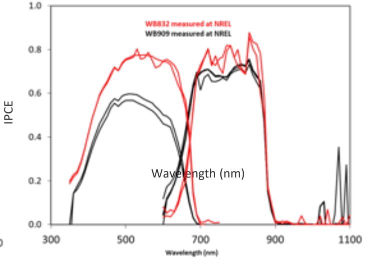


Reproducibility achieved at both Labs

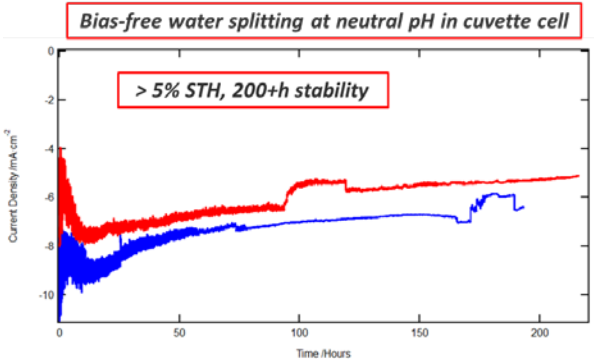








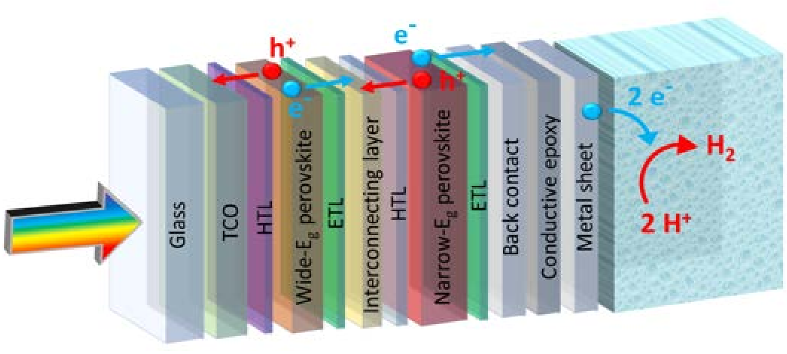
Progress to Date



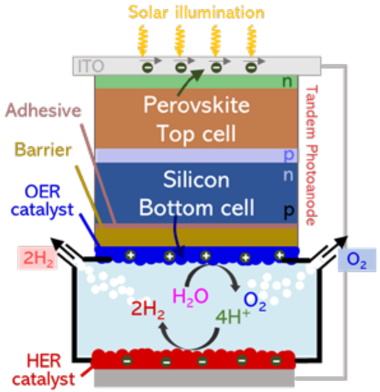
Cathode: *two electrodes from growth # WC106 of GaInP/GaAs III-V tandem, with PtRu catalyst*
Cathode active area: *0.2 cm²*
Anode*: IrOx, separated from the photocathode via Ti mesh*
Electrolyte*: pH 7.2 potassium phosphate remains at neutral pH in bulk throughout 200 hours*
Measurement vessel*: cuvette cell*

HydroGEN PEC Seedling Projects with Lab Capability Support

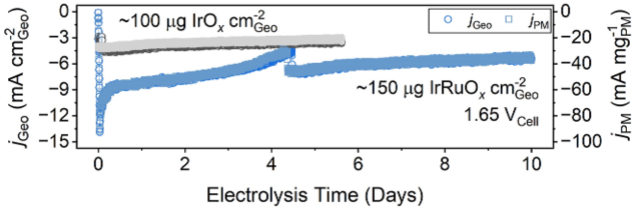
- (U. Toledo, NREL) All-perovskite tandem photoelectrodes for unassisted solar hydrogen production: Perovskite/perovskite tandem photoelectrodes deliver an unbiased STH >18% in a two-electrode configuration under one sun illumination for more than 500 hours.

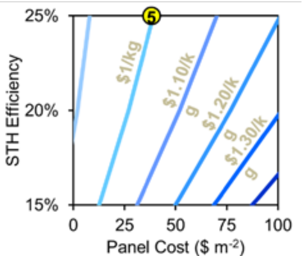


- (Rice, NREL, LBNL) Integrated halide perovskite photoelectrochemical cells with solar-driven water-splitting efficiency of 20.8% : Use of corrosion resistant barrier layers including hydrophobic polymers and ALD oxides enables >100 hours of continuous 1-sun operation at STH > 20%.



Towards earth abundant OER catalysts



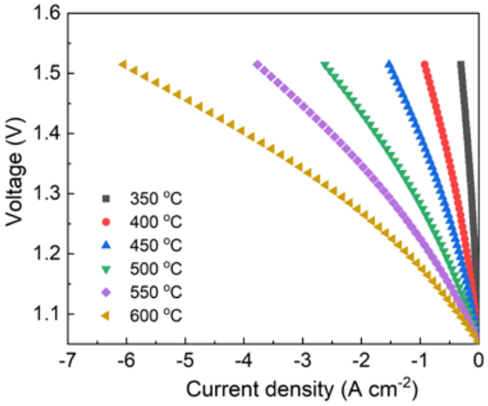


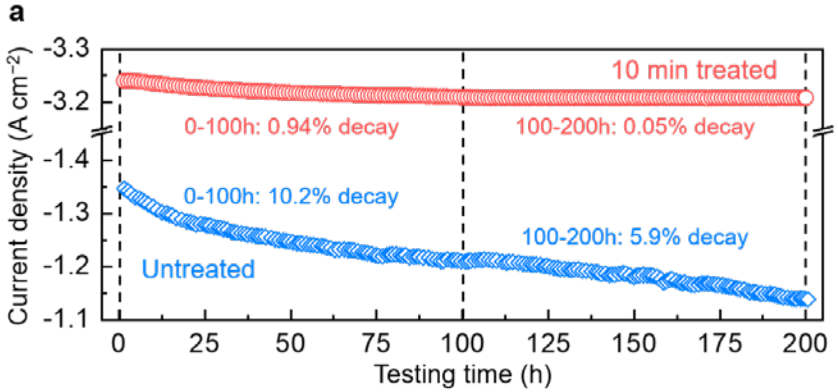
Record performance of p-SOEC with smaller overpotential and lower operating temperatures

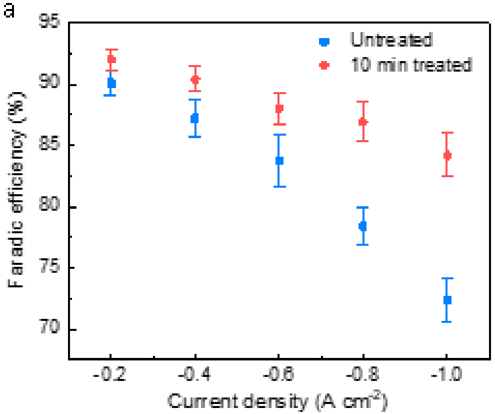
HTE Lab R&D p-SOEC Accomplishments

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



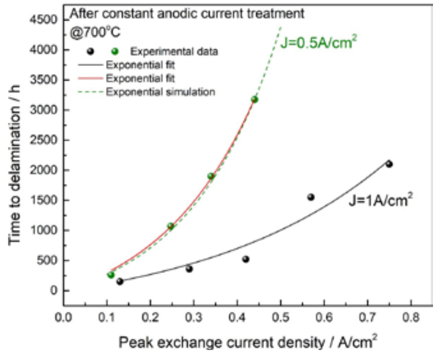




W Bian, W. Wu, D Ding, et al. Nature, 2022

HydroGEN HTE Seedling Projects with Lab Capability Support

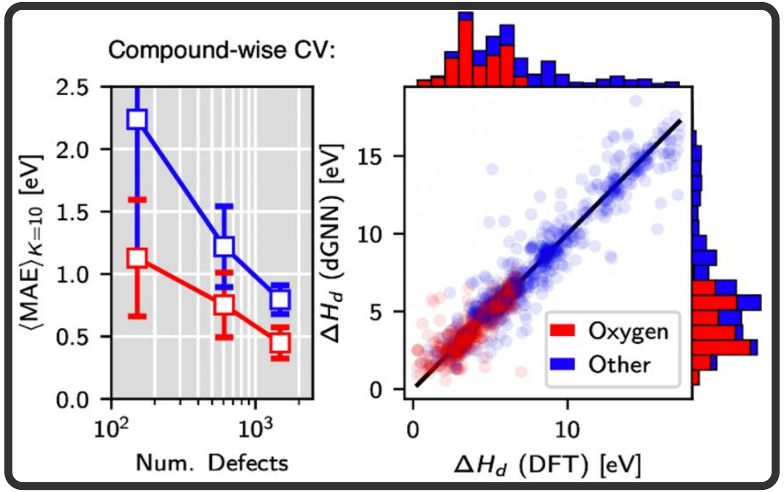
- **(USC, INL and NREL) A Multifunctional Isostructural Bilayer Oxygen Evolution Electrode for Durable Intermediate-Temperature Electrochemical Water Splitting**: Demonstrated a 700^{o}C-bilayer oxygen electrode for solid oxide electrolyzers; Established the relationship between exchange current density and time-to-delamination of oxygen electrode for prediction of safe operating current density; Demonstrated high performance of tubular solid oxide electrolyzers.



- **(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.

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

STCH Lab R&D Accomplishments

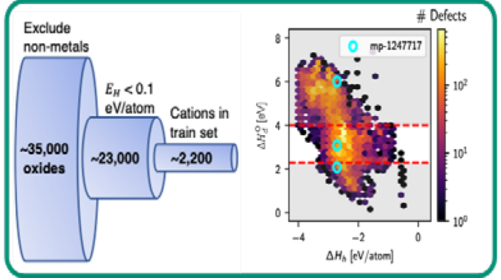


ML screens 10,000's of MP structures in minutes that would take 1,000's of DFT months

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

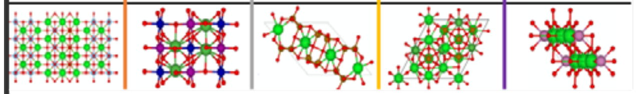
Metric	Requirement
Frac. of defects w/ΔH_d^O > 2.3 eV	x_{min} = 1
Frac. of defects w/$\Delta H_d^O \in$ [2.3, 4.0] eV	x_{rng} > 0
STCH operating range conditions (P_{O_2})	$\Delta\mu'_{O_2}$
Compound stability range	$\Delta\mu_{O_2}^{\phi_H < \{0, 0.1, ...\}}$
Stable in the target range	$\Delta\mu_{O_2}^{\phi_H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

(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)
➢ $x_{min,1} = 1$ ➢ $x_{rng,1} > 0$ ➢ $\Delta\mu_{O_2}^{\phi_H<0.1}$	➢ $x_{min,2} = 1$ ➢ $x_{rng,2} > 0$ ➢ $\Delta\mu_{O_2}^{\phi_H<0.1}$	➢ $x_{min,3} = 1$ ➢ $x_{rng,3} > 0$ ➢ $\Delta\mu_{O_2}^{\phi_H<0.05}$	➢ $x_{min,3} = 1$ ➢ $x_{rng,3} > 0$ ➢ $\Delta\mu_{O_2}^{\phi_H=0}$	➢ $x_{min,3} = 1$ ➢ $x_{rng,3} = 1$ ➢ $\Delta\mu_{O_2}^{\phi_H=0}$
$Sr_6Ti_5FeO_{14}$ (mp-1645141)	La_2MnCoO_6 (mp-19208)	$BaSr(FeO_2)_4$ (mp-1228024)	$Ba_5SrLa_2Fe_4O_{15}$ (mp-698793)	$Ba_3In_2O_6$ (mp-20352)



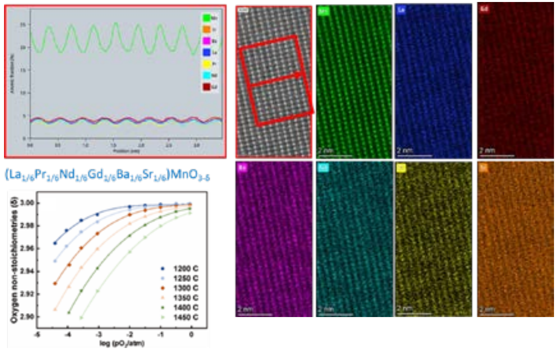
- Identify all candidates satisfying minimum requirements
- Identify candidates with increasingly certain performance
- Mainly IDs known, synthesizable compounds

- 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.

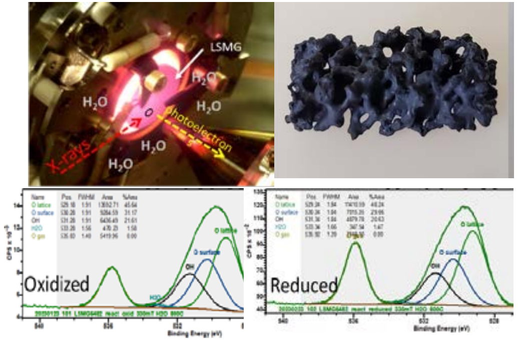
MAE = mean absolute error
MP = Materials Project (https://materialsproject.org/)

HydroGEN STCH Seedling Projects with Lab Capability Support

- **(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.



- **(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.



Community Approach to Benchmarking and Protocol Development for AWS Technologies

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

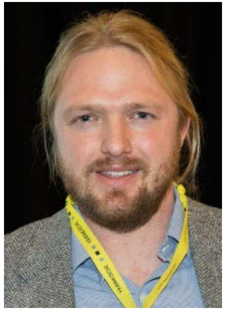
Accomplishments:

- **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
- **5 Annual AWS community-wide benchmarking workshop**
- **Developed high-level roadmaps by AWS technology**

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

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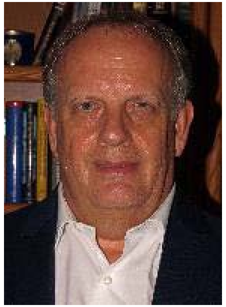
Katie Randolph



Ned Stetson

Eric Miller

NREL/PR-5900-87830