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The #H2IQ Hour

Today's Topic:

HydroGEN Advanced Water Splitting Materials Capabilities Overview

This presentation is part of the monthly H2IQ hour to highlight hydrogen and fuel cell research, development, and demonstration (RD&D) activities including projects funded by U.S. Department of Energy's Hydrogen and Fuel Cell Technologies Office (HFTO) within the Office of Energy Efficiency and Renewable Energy (EERE).

Housekeeping

This webinar is being recorded.

This webinar is being recorded and will be available on the H2IQ webinar archives.

Technical Issues:

- If you experience technical issues, **please check your audio settings under the "Audio" tab.**
- If you continue experiencing issues, direct message the host, Natasha Nguyen

Questions?

There will be a Q&A session at the end of the presentation.

To submit a question, please type it into the **Q&A box on the right-hand side of your screen next to the chat box/Chat**

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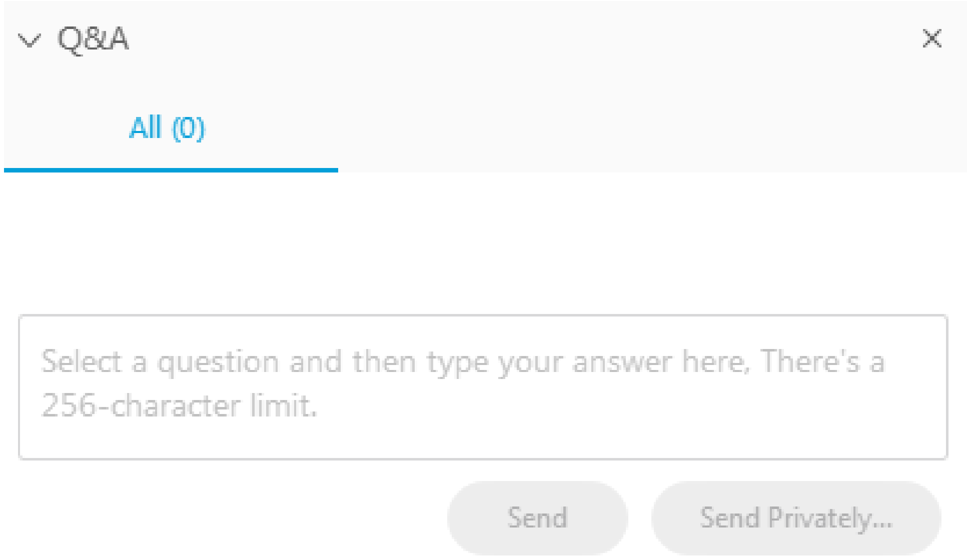
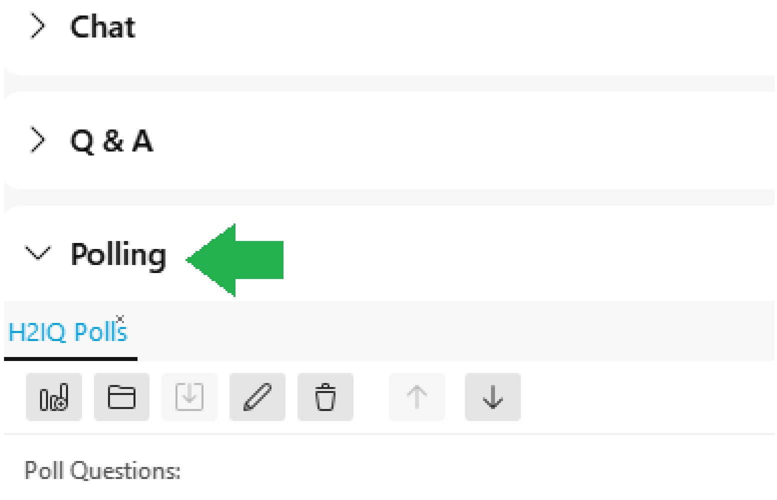
The #H2IQ Hour Q&A

Please type your questions into the **Q&A Box**



#H2IQ Hour Polling Questions

Please submit your answers to our polling questions in the **Polling** Box



Energy Materials Network
U.S. Department of Energy

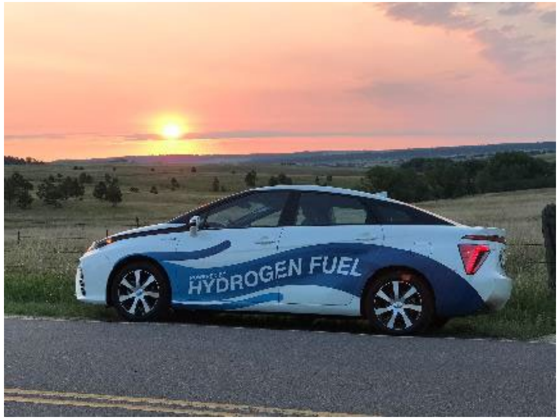
HydroGEN
Advanced Water Splitting Materials

HydroGEN Overview:
A Consortium on Advanced Water Splitting Materials

Huyen Dinh, Director of HydroGEN, NREL

9/16/2022, Virtual

H2IQ HydroGEN EMN Webinar



NREL Transforming ENERGY

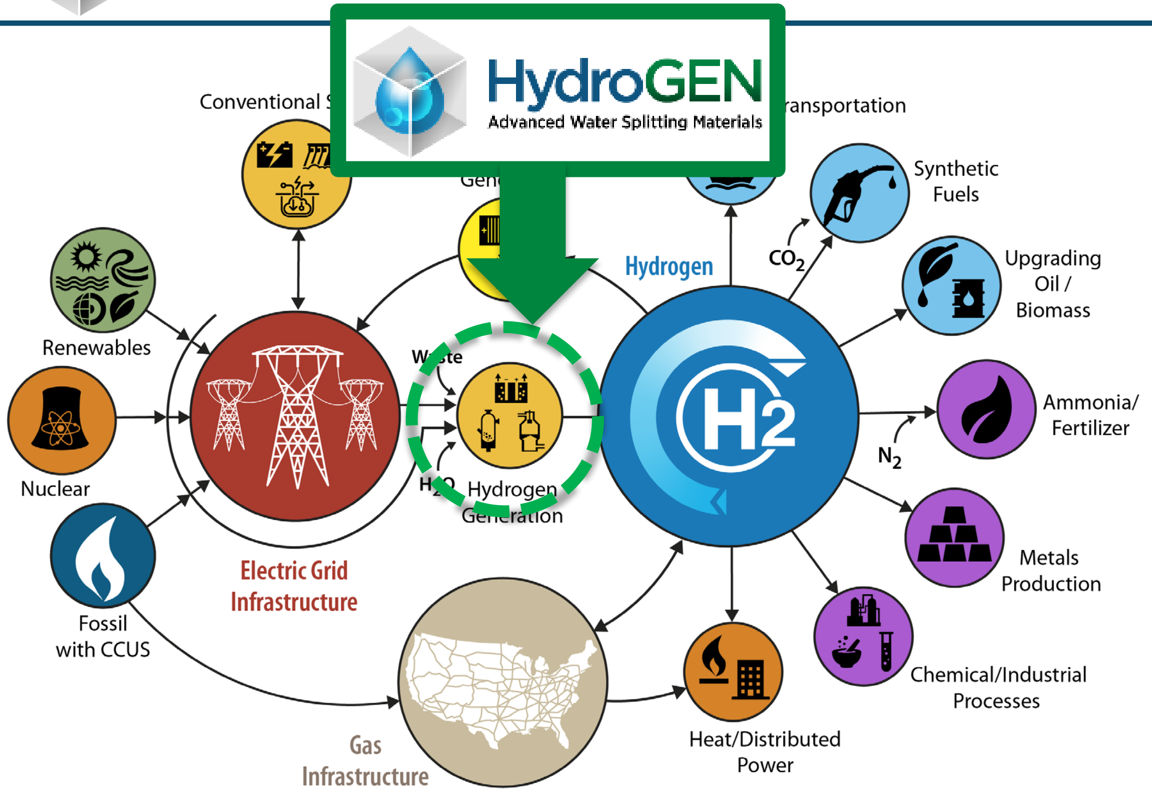
BERKELEY LAB Bringing Science Solutions to the World

Sandia National Laboratories

INL Idaho National Laboratory

Lawrence Livermore National Laboratory

H2@Scale: Enabling affordable, reliable, clean and secure energy



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

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

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

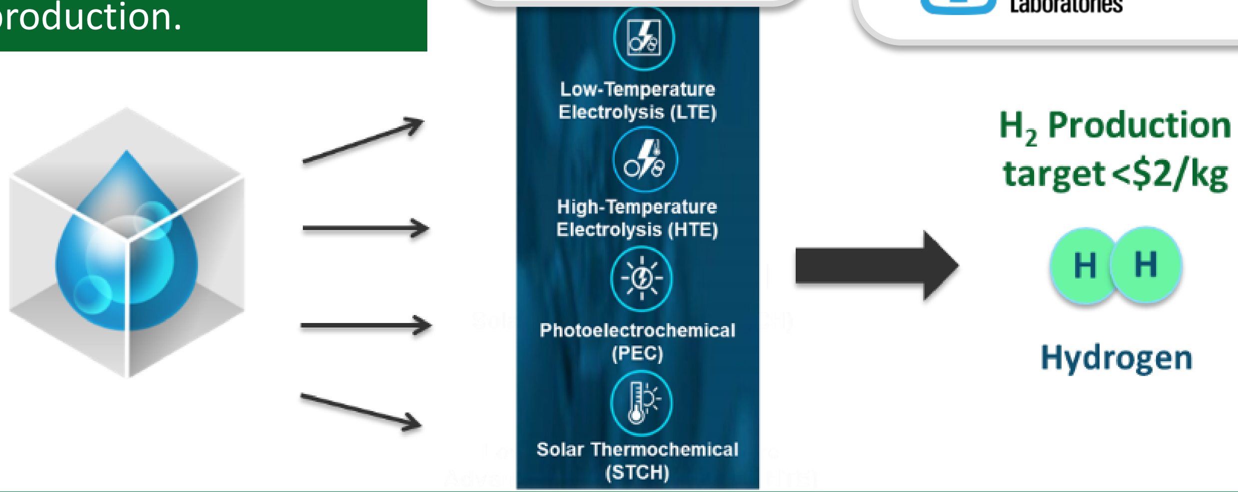
Goal: Accelerating R&D of innovative advance water splitting (AWS) materials and technologies for clean, sustainable and low-cost hydrogen production.

Barriers

- Cost
- Efficiency
- Durability

National Lab Consortium Team

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

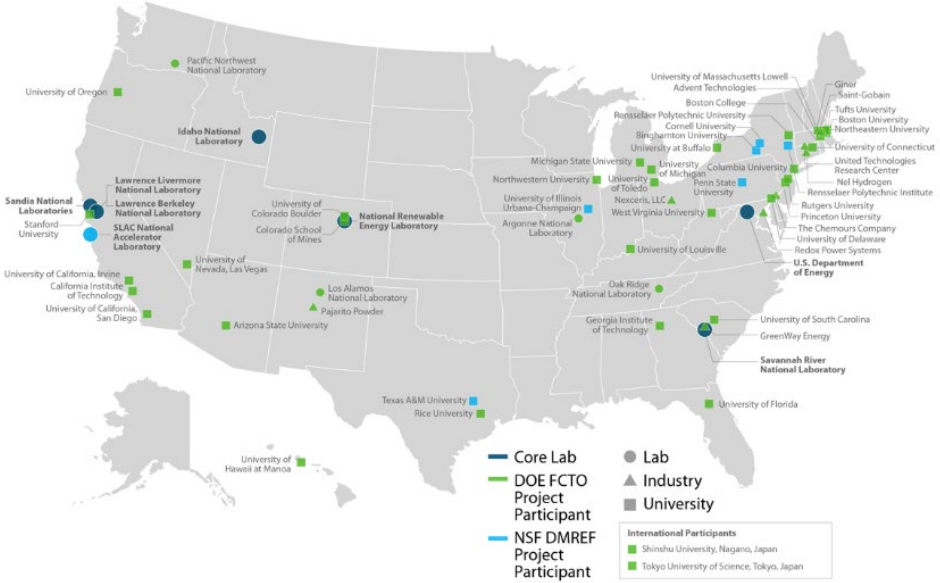


HydroGEN is advancing Hydrogen Shot goals by fostering cross-cutting innovation using theory-guided applied materials R&D to advance all emerging water-splitting pathways for hydrogen production

HydroGEN EMN Framework

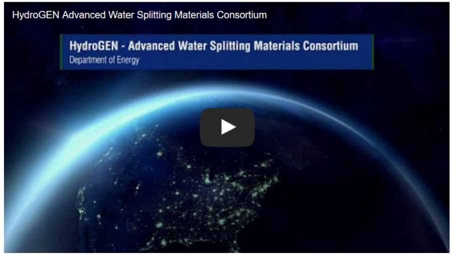
Collaboration, Streamline Access

11 Labs **10** Companies **39** Universities **2** Funding Agencies



Non-Disclosure Agreement (NDA)	Intellectual Property Management Plan (IPMP)	Materials Transfer Agreement (MTA)	Cooperative Research and Development Agreement (CRADA)
Information Disclosure	IP Protection	Freedom to Operate	Collaboration

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



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

2 R&D 100 Awards

118 Publications, Impact factor* = 2.20
2,783 citations, 436 authors

4 community benchmarking workshops

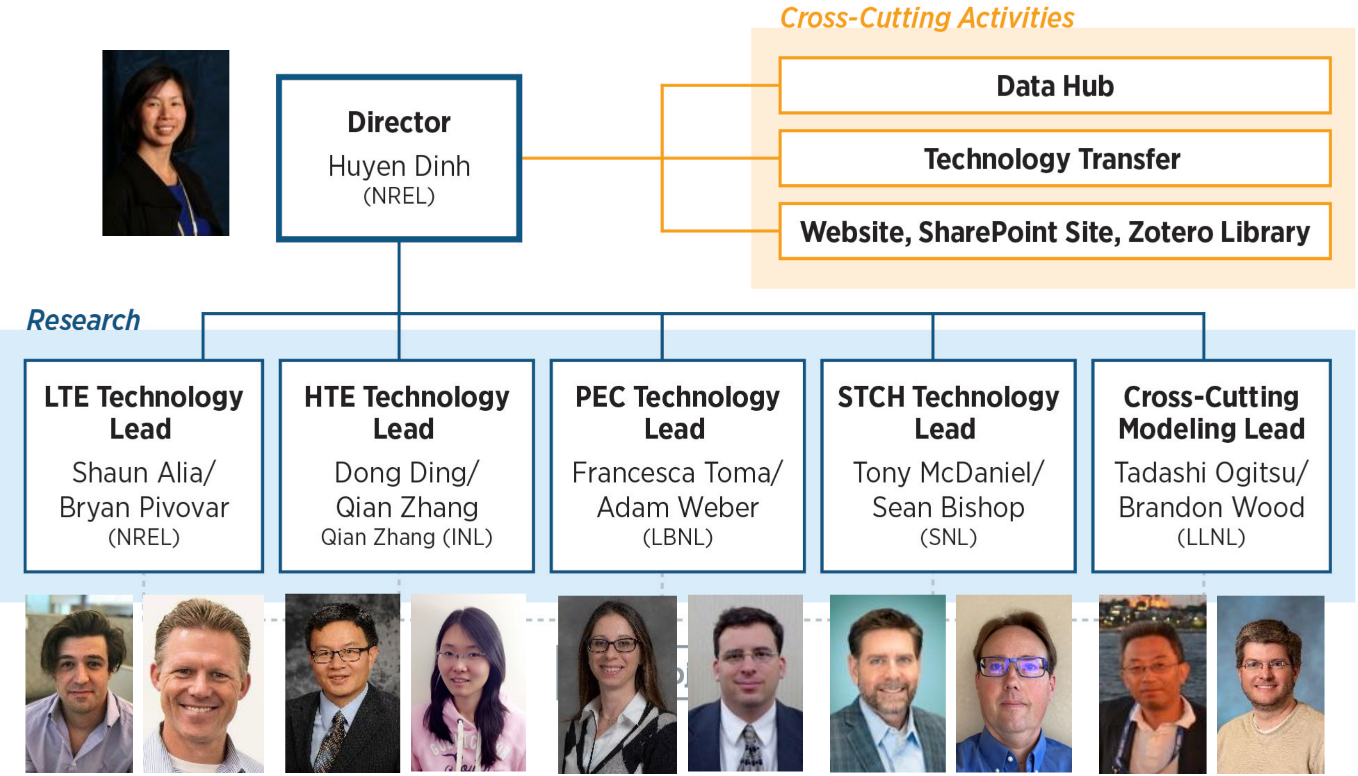
33 project NDAs, 2 MTAs

46 capabilities utilized across 6 labs

STEM Work Force Development

*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.

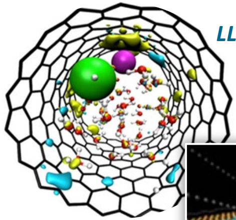
Diverse HydroGEN Leadership and Community



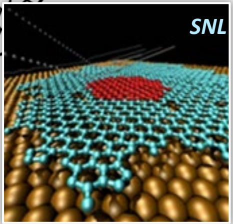
HydroGEN-AWSM Consortium Capabilities Network

Comprising more than 60 unique, world-class capabilities/expertise in:

Materials Theory/Computation

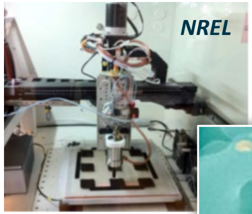


Bulk & interfacial models of aqueous electrolytes

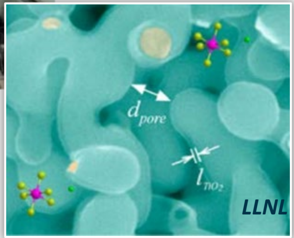


LAMMPS classic molecular dynamics modeling relevant to H_2O splitting

Advanced Materials Synthesis



High-throughput spray system for electrode fabrication



Conformal ultrathin TiO_2 ALD coating on bulk nanoporous gold

Characterization & Analytics

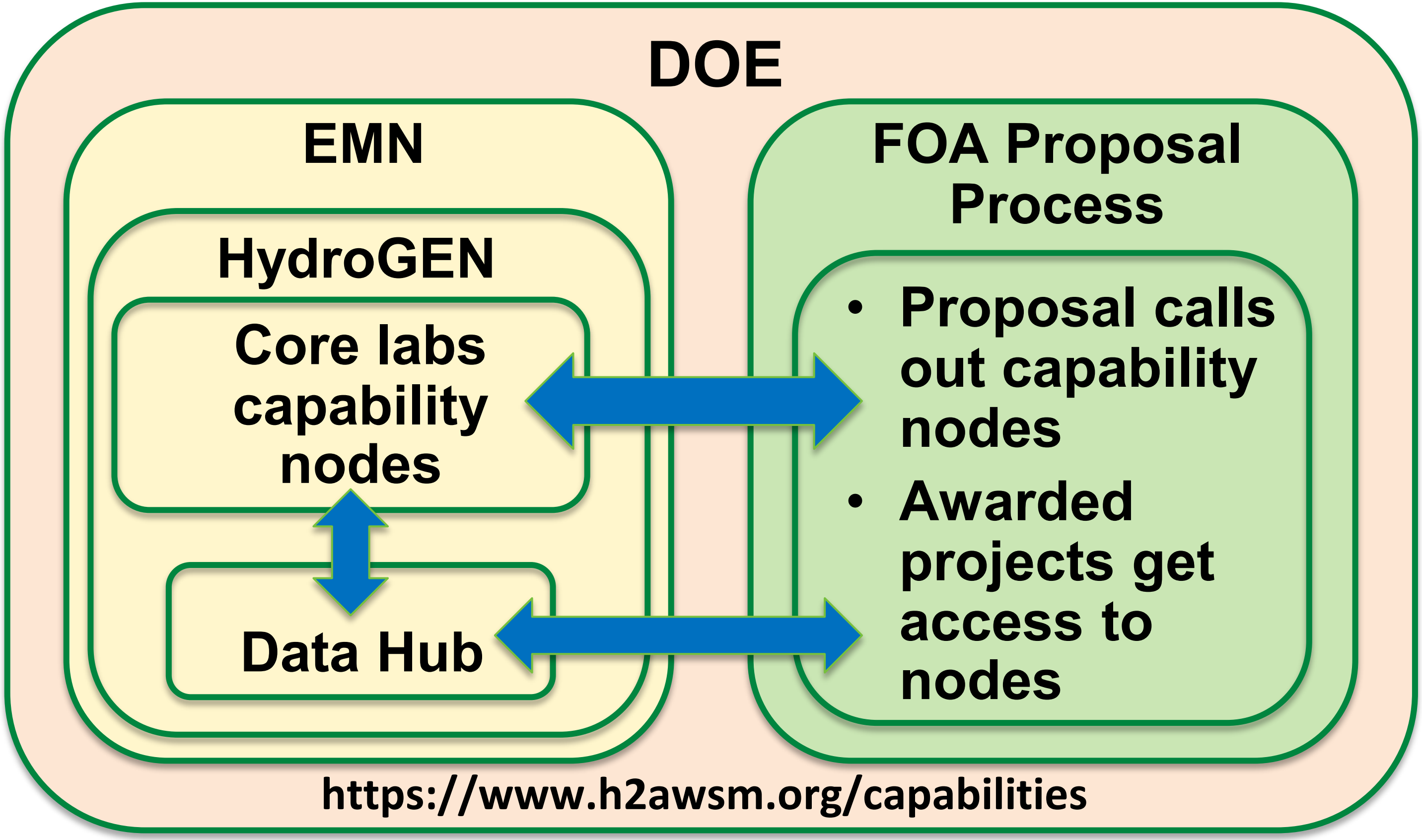
Stagnation flow reactor to evaluate kinetics of redox material at high-T

TAP reactor for extracting quantitative kinetic data

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

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

HydroGEN EMN Collaborates with Projects



HydroGEN Labs Support FOA-Awarded Projects

STCH Node Labs

Sandia National Laboratories

INL Idaho National Laboratory

NREL NATIONAL RENEWABLE ENERGY LABORATORY

SRNL SAVANNAH RIVER NATIONAL LABORATORY

Lawrence Livermore National Laboratory

Support through:

Personnel

Equipment

Expertise

Capability

Materials

Data

STCH FOA Projects

ASU Arizona State University

COLORADO SCHOOL OF MINES

CU

Northwestern University

UCSD

UF UNIVERSITY of FLORIDA

Greenway Energy LLC

Engineering consultant in Aiken County, South Carolina

Capability Nodes on the User-Friendly Node Search Engine for Stakeholders

> 60 current capability nodes

- 44 PEC capabilities
- 28 STCH capabilities
- 39 LTE capabilities
- 35 HTE capabilities
- 7 Hybrid thermal (HT) capabilities

Node Readiness Category (NRC) Chart

1	Node is **fully developed** and has been used for AWSM research projects
2	Node requires **some development** for AWSM
3	Node requires **significant development** for AWSM

Search

Reset filtering

CAPABILITY CLASS

- Analysis
- Benchmarking
- Characterization
- Computational Tools and Modeling
- Data Management
- Material Synthesis
- Process and Manufacturing Scale-Up
- System Integration

WATER-SPLITTING TECHNOLOGY

High-Temperature Electrolysis
- HTE 1 - HTE 2 - HTE 3

Low-Temperature Electrolysis
- LTE 1 - LTE 2 - LTE 3

Photoelectrochemical
- PEC 1 - PEC 2 - PEC 3

Solar Thermochemical
- STCH 1 - STCH 2 - STCH 3

Hybrid Thermochemical
- HT 1 - HT 2 - HT 3

Node Readiness Categories

NATIONAL LABORATORY

- Idaho National Laboratory (INL)
- Lawrence Berkeley National Laboratory (LBNL)
- Lawrence Livermore National Laboratory (LLNL)
- National Renewable Energy Laboratory (NREL)
- Sandia National Laboratories (SNL)

Show 12 Apply

Reset

Stakeholders can search for relevant materials synthesis, characterization, analysis, and modeling capabilities to meet their needs

HydroGEN Capabilities Website/Search Engine - Demo

Demo

LIST OF CAPABILITIES

Each capability represents a resource node—a combination of a tool, technique, and expertise—that is unique to the national laboratory system. Each resource node is assigned a node readiness category that describes the readiness of the capability node for use in the water splitting pathway listed.

NATIONAL LABORATORY

- ☐ Idaho National Laboratory (INL)
- ☐ Lawrence Berkeley National Laboratory (LBNL)
- ☐ Lawrence Livermore National Laboratory (LLNL)
- ☐ National Renewable Energy Laboratory (NREL)
- ☐ Sandia National Laboratories (SNL)

Show

12 | Apply

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Search

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CAPABILITY CLASS

- ☐ Analysis
- ☐ Benchmarking
- ☐ Characterization
- ☐ Computational Tools and Modeling
- ☐ Material Synthesis
- ☐ Process and Manufacturing Scale-Up
- ☐ System Integration

WATER-SPLITTING TECHNOLOGY

High-Temperature Electrolysis
☐ HTE 1 ☐ HTE 2 ☐ HTE 3

Low-Temperature Electrolysis
☐ LTE 1 ☐ LTE 2 ☐ LTE 3

Photoelectrochemical
☐ PEC 1 ☐ PEC 2 ☐ PEC 3

Solar Thermochemical
☐ STCH 1 ☐ STCH 2 ☐ STCH 3

Hybrid Thermochemical
☐ HT 1 ☐ HT 2 ☐ HT 3

Node Readiness Categories

Showing 1 to 12 of 63 entries

1 2 3 4 Next

Capability	Lab	Nodes
Ab Initio Modeling of Electrochemical Interfaces	LLNL	LTE 2, PEC 1
Advanced Electrode and Solid Electrolyte Materials for Elevated Temperature Water Electrolysis	INL	HTE 1
Advanced Electron Microscopy	SNL	HTE 2, LTE 2, PEC 2, STCH 1
Albany: Open-Source Multiphysics Research Platform	SNL	HTE 3, LTE 3, PEC 3, STCH 2
ALD Based Surface Functionalization and Porosity Control	LLNL	PEC 3
Analysis and Characterization of Hydrided Material Performance	INL	HTE 2
Beyond-DFT Simulation of Energetic Barriers and Photoexcited Dynamics	LLNL	PEC 2
Characterization of Semiconductor Bulk and Interfacial Properties and On-Sun Photoelectrochemical So...	NREL	PEC 1
Characterizing Degradation Processes at Photoelectrochemically Driven Interfaces	LLNL	PEC 1, LTE 2

STCH: Characterization Capabilities - Demo

Search

Reset filtering

CAPABILITY CLASS

- [ ] Analysis
- [ ] Benchmarking
- [x] Characterization
- [ ] Computational Tools and Modeling
- [ ] Material Synthesis
- [ ] Process and Manufacturing Scale-Up
- [ ] System Integration

WATER-SPLITTING TECHNOLOGY

High-Temperature Electrolysis

- [ ] HTE 1
- [ ] HTE 2
- [ ] HTE 3

Low-Temperature Electrolysis

- [ ] LTE 1
- [ ] LTE 2
- [ ] LTE 3

Photoelectrochemical

- [ ] PEC 1
- [ ] PEC 2
- [ ] PEC 3

Solar Thermochemical

- [x] STCH 1
- [ ] STCH 2
- [ ] STCH 3

Hybrid Thermochemical

- [ ] HT 1
- [ ] HT 2
- [ ] HT 3

Node Readiness Categories

Advanced Electron Microscopy	SNL	HTE 2, LTE 2, PEC 2, STCH 1
Concentrating Solar Power Furnace	SNL	HTE 2, PEC 2, STCH 1, HT 1
Controlled Materials Synthesis and Defect Engineering	NREL	HTE 2, STCH 1
High Flux Solar Furnace	NREL	STCH 1, HTE 2
High-Temperature X-Ray Diffraction (HT-XRD) and Complementary Thermal Analysis	SNL	HTE 1, LTE 1, PEC 1, STCH 1, HT 1
Photoelectrochemical Device In Situ and Operando Testing Using X-Rays	LBNL	HTE 1, LTE 1, PEC 1, STCH 1
Virtually Accessible Laser Heated Stagnation Flow Reactor for Characterizing Redox Chemistry of Mate...	SNL	STCH 1

Showing 1 to 7 of 7 entries

PEC: Characterization Capabilities - Demo

Search

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CAPABILITY CLASS

- [ ] Analysis
- [ ] Benchmarking
- [x] Characterization
- [ ] Computational Tools and Modeling
- [ ] Material Synthesis
- [ ] Process and Manufacturing Scale-Up
- [ ] System Integration

WATER-SPLITTING TECHNOLOGY

High-Temperature Electrolysis

- [ ] HTE 1 - [ ] HTE 2 - [ ] HTE 3

Low-Temperature Electrolysis

- [ ] LTE 1 - [ ] LTE 2 - [ ] LTE 3

Photoelectrochemical

- [x] PEC 1 - [ ] PEC 2 - [ ] PEC 3

Solar Thermochemical

- [ ] STCH 1 - [ ] STCH 2 - [ ] STCH 3

Hybrid Thermochemical

- [ ] HT 1 - [ ] HT 2 - [ ] HT 3

Node Readiness Categories

NATIONAL LABORATORY

- [ ] Idaho National Laboratory (INL)
- [ ] Lawrence Berkeley National Laboratory (LBNL)
- [ ] Lawrence Livermore National Laboratory (LLNL)
- [ ] National Renewable Energy Laboratory (NREL)
- [ ] Sandia National Laboratories (SNL)

Showing 1 to 12 of 13 entries   1 2 Next

Capability	Laboratory	Technology
Characterization of Semiconductor Bulk and Interfacial Properties and On-Sun Photoelectrochemical So...	NREL	PEC 1
Characterizing Degradation Processes at Photoelectrochemically Driven Interfaces	LLNL	PEC 1, LTE 2
Corrosion Analysis of Materials	NREL	HTE 3, LTE 1, PEC 1
Electron Beam and In Situ Photon Beam Characterization of PEC Materials and Devices	SNL	LTE 2, PEC 1
High-Temperature X-Ray Diffraction (HT-XRD) and Complementary Thermal Analysis	SNL	HTE 1, LTE 1, PEC 1, STCH 1, HT 1
I-III-VI Compound Semiconductors for Water Splitting	NREL	PEC 1
In Situ/Operando X-Ray Characterization of Electronic Structure in Photoabsorber Materials	LLNL	PEC 1, LTE 2
Laboratory and On-Sun PEC Device Testing	LBNL	PEC 1
Photoelectrochemical Device In Situ and Operando Testing Using X-Rays	LBNL	HTE 1, LTE 1, PEC 1, STCH 1
Probing and Mitigating Chemical, Electrochemical, and Photochemical Corrosion of Electrochemical and...	LBNL	HTE 2, LTE 2, PEC 1
Surface Analysis Cluster Tool	NREL	HTE 2, LTE 1, PEC 1, STCH 2
Surface Modifications for Catalysis and Corrosion Mitigation	NREL	LTE 1, PEC 1

Showing 1 to 12 of 13 entries   1 2 Next

Characterization of Semiconductor Bulk and Interfacial Properties and On-Sun Photoelectrochemical Solar-to-Hydrogen Benchmarking

LABORATORY	CAPABILITY EXPERT	CLASS	NODE READINESS CATEGORY
National Renewable Energy Laboratory (NREL)	Todd Deutsch, James Young	Benchmarking Characterization	1: Photoelectrochemical (PEC)

DESCRIPTION

Characterization of Semiconductor Bulk and Interfacial Properties

This capability involves characterizing semiconductors using photoelectrochemical (PEC) methods to measure their bulk and interfacial properties to determine their suitability for photoelectrolysis. We have practical experience contacting a variety of semiconductor configurations and fabricating samples into photoelectrodes suitable for PEC testing. Once we fabricate electrodes and measure their surface areas, we use a suite of characterization methods to determine unknown semiconductor properties by the following procedure:

1. We determine the conductivity type of an unknown material by monitoring the open-circuit potential response upon illumination, which is important to establish the reverse-bias conditions used for all subsequent testing.
2. We then measure band gap energy to within ±0.01 eV as well as determine whether the electronic transition is direct or indirect with our custom-built photocurrent spectroscopy system.
3. Once the bandgap is known, we use the appropriate reference cells and calibrated light sources to measure (photo)current-potential performance under simulated reference illumination (AM1.5 G).
4. We then determine the conduction/valence band edge alignment by measuring the flatband potential across a range of electrolytes with varying pHs using three different techniques; photocurrent onset, VOC under intense illumination, and Mott-Schottky analysis.
5. The doping density of the semiconductor is calculated from the slope of the Mott-Schottky response.
6. We measure incident photon-to-current efficiency (IPCE) to get a wavelength-dependent conversion efficiency that can be integrated over a reference spectrum (AM1.5G) to corroborate the photocurrents obtained under broadband illumination.
7. The reflectance may also be monitored during the IPCE measurement to calculate wavelength-dependent internal quantum efficiency.

Efficiency Benchmarking

This capability involves testing water-spitting semiconductors and semiconductor-based devices using simulated and actual solar (on-sun) illumination to validate solar-to-hydrogen (STH) conversion efficiency. The first step is to take incident photon-to-current efficiency measurements to get the wavelength dependent conversion efficiency for each subcell absorber junction. This is necessary to calculate a spectral correction factor to adjust measured photocurrent densities to a reference spectrum for objective comparison of performance to other devices. Outdoor measurements are taken using collimating tubes to isolate the direct component of the solar spectrum to minimize errors due to coupling of the diffuse component of solar radiation to the semiconductor by the photoreactor cell. Continuous research-quality measurements of the characteristics of local solar irradiance are recorded at the Solar Radiation Research Laboratory (SRRL) at NREL every minute from over 80 instruments including pyranometers, pyroheliometers, pyrgeometers, anemometers and other meterological sensors. Details on the measurements and data sets are online. This data is used to calculate real-time STH efficiencies from short-circuit current density measurements

CAPABILITY BOUNDS

Custom cells may be required to accommodate various electrode geometries. Electrode sizes from 0.01 cm2 up to several cm2 can be tested.

UNIQUE ASPECTS

These semiconductor characterization techniques have been funded by the Hydrogen & Fuel Cell Technologies Office for >20 years. We have trained dozens of undergraduate, graduate, and postdoctoral researchers and tested thousands of c-Si, a-Si, oxide, nitride, carbide, phosphide, arsenide, selenide, sulfide, bismide, and antimonide semiconductors and co-authored a book based on our approach. What sets the efficiency benchmarking capability apart from other benchmarking facilities is the colocation of STH testing with the collection of solar radiation data at SRRL, the home of the world's largest collection of radiometers in continuous operation dating back to 1981. Another unique characteristic of this capability is its extraordinary availability due to the excellent solar access intrinsic to Colorado.

AVAILABILITY

We have 5-6 characterization stations that include potentiostats, frequency response analyzers, and light sources permitting a relatively high PEC characterization throughput. A scientist unskilled in this area could gain moderate proficiency on these characterization techniques within a few days of training. Its high availability would allow this capability to serve as a user facility if a large number of sample characterizations is needed. Long-term STH efficiency testing is limited by availability of the tracker that can vary based on demand. Dozens of short-term STH efficiency measurements can be performed daily but are weather dependent. Additional rooftop space at the Energy Systems Integration Facility is designated for on-sun STH benchmarking and long-term testing.

BENEFIT

This capability can screen unknown photoelectrode candidate materials and, by evaluating their intrinsic bulk and interfacial properties, determine their potential to direct sunlight toward water splitting. The co-location of all measurement equipment and capability experts offers convenience, support, and quick turnaround for users. This capability can also verify/certify solar conversion into hydrogen under true solar conditions that are difficult to accurately measure using simulated laboratory conditions, especially for the multijunction systems capable of the highest STH efficiencies.

IMAGES

REFERENCES

1. "Accelerating materials development for photoelectrochemical (PEC) hydrogen production: Standards for methods, definitions, and reporting protocols" Zhebo Chen, Thomas F. Jaramillo, Todd G. Deutsch, Alan Kleiman-Shwarsctein, Arnold J. Forman, Nicolas Gaillard, Roxanne Garland, Kazuhiro Takanabe, Clemens Heske, Mahendra Sunkara, Eric W. McFarland, Kazunari Domen, Eric L. Miller, John A. Turner, Huyen N. Dinh, J. Mater. Res. 25(1), 3-16 (2010).

2. Photoelectrochemical Water Splitting: Standards, Experimental Methods, and Protocols, Zhebo Chen, Huyen N. Dinh, Eric Miller, Todd G. Deutsch, Kazunari Domen, Keith Emery, Arnold J. Forman, Nicolas Gaillard, Roxanne Garland, Clemens Heske, Thomas F. Jaramillo, Alan Kleiman-Shwarsctein, Kazuhiro Takanabe, John Turner, eds: Zhebo Chen, Huyen N. Dinh, Eric Miller. New York: Springer, 2013.

3. "Photoelectrochemical Characterization and Durability Analysis of GaInPN Epilayers" Todd G. Deutsch, Jeff L. Head, John A. Turner. J. Electrochem. Soc. 155(9) B903, (2008).

4. "Solar to hydrogen efficiency: Shining light on photoelectrochemical device performance," H. Döscher, J.L. Young, J.F. Geisz, J.A. Turner, T.G. Deutsch, Energy Environ. Sci., 9, 74-80 (2016).

5. "Direct solar-to-hydrogen conversion via inverted metamorphic multi-junction semiconductor architectures" James L. Young, Myles A. Steiner, Henning Döscher, Ryan M. France, John A. Turner, and Todd G. Deutsch, Nature Energy 2, 17028 (2017).

6. "Translation of device performance measurements to reference conditions." C. R. Osterwald, Solar Cells, 18, 269–279 (1986).

J. Electrochem. Soc. 155, no. 9 (2008): B903.

HydroGEN Capability Nodes By Water Splitting Technologies/Projects

(LTE, HTE, PEC, STCH projects)

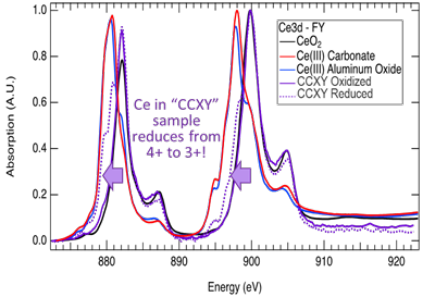
HydroGEN Capability Node	Node Class	LTE	HTE	PEC	STCH
LBNL Multiscale Modeling of Water Splitting Devices	Modeling	✓			
INL Advanced Materials for Elevated Temperature Water Electrolysis	Characterization		✓		
NREL In-Situ Testing Capabilities for Hydrogen Generation	Characterization	✓			
NREL Thin Film Combinatorial Capabilities for Advanced Water Splitting Technologies	Synthesis + Characterization		✓	✓	✓
NREL First Principles Materials Theory for Advanced Water Splitting Pathways	Modeling				✓
NREL On-Sun PEC Solar-to-Hydrogen Benchmarking	Characterization			✓	
LBNL Thin Film and Bulk Ionomer Characterization	Characterization	✓			
SNL High-Temperature X-ray Diffraction and Thermal Analysis	Characterization		✓		✓
NREL Multi-Component Ink Development, High Throughput Fabrication, and Scaling Studies	Processing & Scale Up	✓			
SNL Virtually Accessible Laser Heated Stagnation Flow Reactor	Characterization				✓
LLNL Ab Initio Modeling of Electrochemical Interfaces	Modeling			✓	✓

ASU Seedling Project: Incorporate Second Redox Active Sublattice to Modify STCH Cycle Thermodynamics

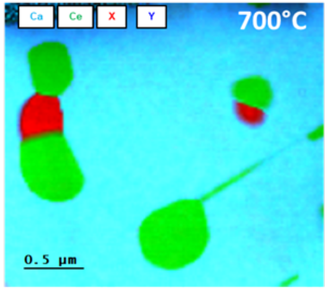
Goal: Computational discovery of STCH materials with simultaneously reduceable cations on separate sublattices.

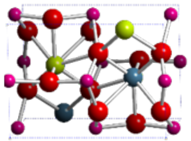
https://www.hydrogen.energy.gov/pdfs/review21/p168_stechel_2021_p.pdf

- Three HydroGEN nodes collaborated with ASU.
  - Controlled Material Synthesis (NREL)
  - Advanced Electron Microscopy (SNL)
  - Virtually Accessible Laser Heated Flow Reactor (SNL)
- NREL: Synthesized and characterized crystal structure and identified redox active cations.
  - Confirmed dual-cation reduction mechanism by XAS
- SNL: Characterized water splitting and A-site cation redox activity.
  - Confirmed $Ce^{(4+/3+)}$ redox in CCXY phase as predicted
  - Confirmed CCXY splits water at low p_{O2}

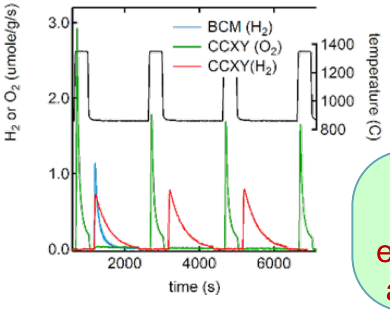


CCXY Phase EDS Map

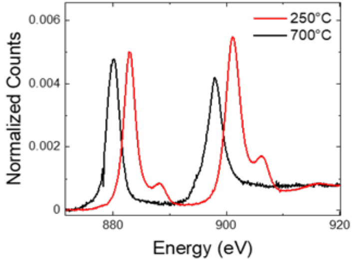




To=850C, 40% H_2O for 1200s, Tr=1350C for 330s



CCXY EELS Ce M-edge



synergy and information exchange between nodes enhanced collaboration with ASU and facilitated project's success

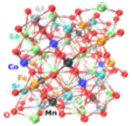
UCSD Seedling Project: High Entropy Perovskite Oxides with Increased Reducibility for STCH

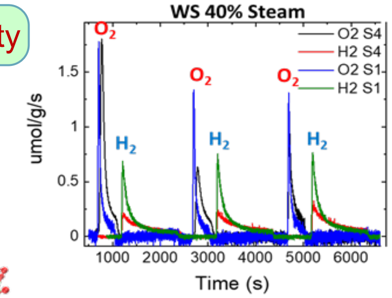
Goal: Modulate oxygen reduction enthalpy and increase oxygen reduction entropy using high entropy perovskites oxides (HEPOs).

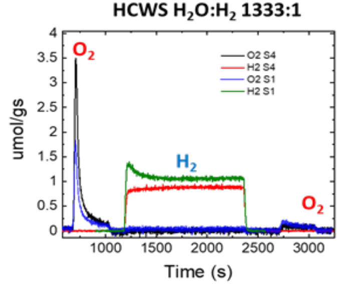
https://www.hydrogen.energy.gov/pdfs/review22/p194_luo_2022_p.pdf

nodes explained why small variation in Co fraction impacts STCH functionality

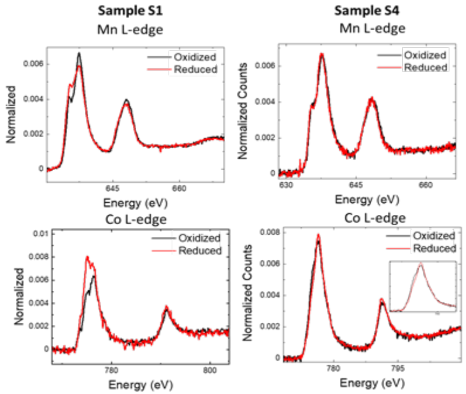
- Three HydroGEN nodes collaborated with UCSD.
  - First Principles Materials Theory (NREL)
  - Advanced Electron Microscopy (SNL)
  - Virtually Accessible Laser Heated Flow Reactor (SNL)
- NREL: Explored configurational disorder via Monte-Carlo simulations of defect structures.
  - Cobalt redox activity modulated by coordination with O vacancies
- SNL: Characterized water splitting and cation redox activity.
  - Small compositional variation greatly impacts redox behavior
  - Dual cation reduction (Mn, Co) observed via EELS



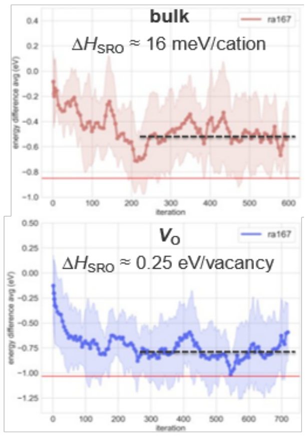




Sample compositions	
HEPO-S1	$(La_{0.8}Sr_{0.2})(Mn_{0.28}Fe_{0.28}Co_{0.16}Al_{0.28})O_3$
HEPO-S4	$(La_{0.8}Sr_{0.2})(Mn_{0.2}Fe_{0.2}Co_{0.4}Al_{0.2})O_3$



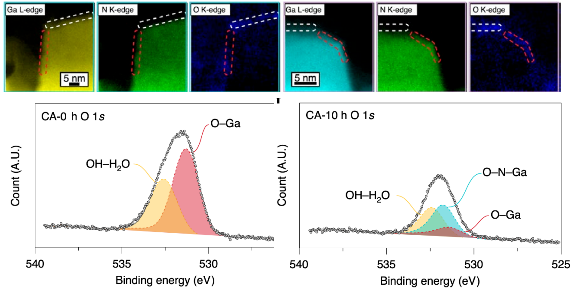
Monte-Carlo simulations



U. Michigan Seedling Project: Monolithically Integrated Thin-Film/Si Tandem Photoelectrodes

Goal: Develop Si-based low cost tandem photoelectrodes to achieve high efficiency (>15%) and stable (>1,000 hrs) water splitting systems. https://www.hydrogen.energy.gov/pdfs/review20/p163_mi_2020_p.pdf

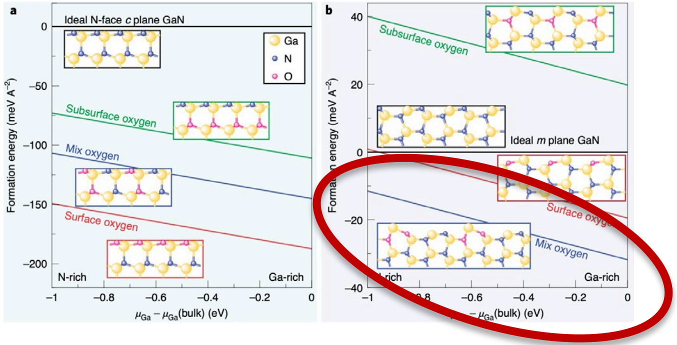
- Three HydroGEN nodes at three National Labs.
  - In situ and operando/Probing corrosion (LBNL)
  - Interface Modeling (LLNL)
  - Surface modification/Surface Analysis (NREL)
- LBNL: Performed microscopy and spectroscopy analysis of the photoelectrodes.
  - Confirmed presence of a new oxynitride species
- LLNL: Performed DFT calculations to understand the stability and activity of the oxynitride phase.
  - substitution of N with O yields the lowest surface free energy among of all the reported GaN m-plane structures
- NREL: Performed co-catalyst deposition on GaN surface to lower kinetic barrier for H_2 evolution



Beginning   After 10 hours

Collaboration enabled discovery of protection mechanism and self-improvement of GaN on Si photocathodes

c-plane   m-plane

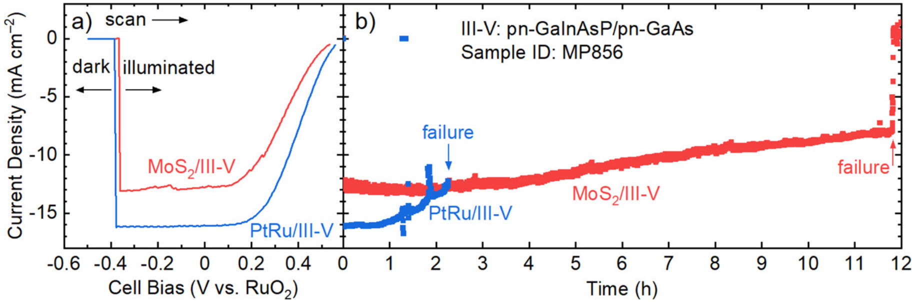


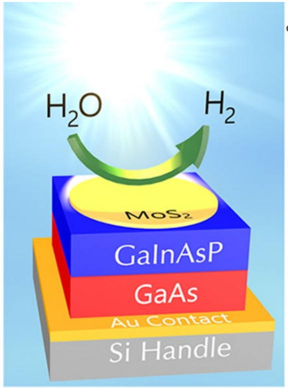
Nature Materials doi.org/10.1038/s41563-021-00965-w

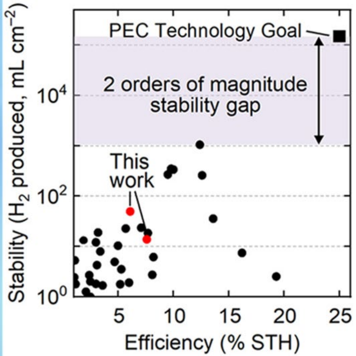
U. Stanford Seedling Project: Protective Catalyst Systems on III-V and Si-based Semiconductors for Efficient, Durable PEC Water Splitting Devices

Goal: To develop unassisted water splitting devices with protective/catalytic MoS_2 barriers for durable, high-efficiency PEC water splitting https://www.hydrogen.energy.gov/pdfs/review21/p161_jaramillo_2021_p.pdf

- Five HydroGEN nodes at two National Labs:
  - III-V Semiconductor Synthesis (NREL)
  - Characterization of bulk and interfacial properties (NREL)
  - Corrosion Analysis of Materials (NREL)
  - On-Sun Efficiency Benchmarking (NREL)
  - Photophysical Characterization (LBNL)
- <u>NREL</u>: Design/synthesis of III-V photocathodes, applied PtRu cocatalysts, evaluated durability, performed on-sun photoreactor tests
- <u>LBNL</u>: Performed transient absorption spectroscopy and in-situ Raman measurements to evaluate band gaps and materials defects







Collaboration achieved 6x greater PEC durability with non-precious MoS_2 catalysts (vs. PtRu)

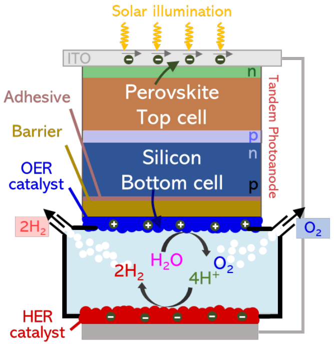
ACS Energy Letters 10.1021/acsenergylett.0c01132

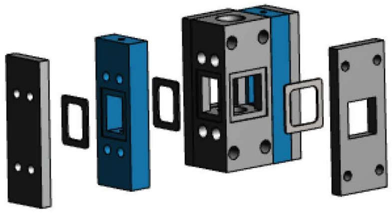
Rice Seedling Project: Highly Efficient Solar Water Splitting Using 3D/2D Hydrophobic Perovskites with Corrosion Resistant Barriers

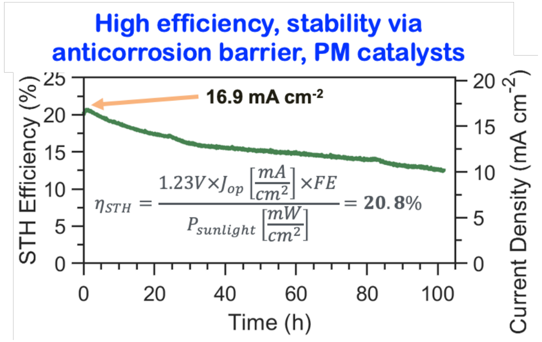
Goal: Develop tandem perovskite absorbers that exceed 20% STH efficiency with low cost and high durability.

https://www.hydrogen.energy.gov/pdfs/review22/p193_mohite_2022_p.pdf

- Three HydroGEN nodes at three National Labs:
  - In situ and operando/Probing corrosion (LBNL)
  - On-Sun Efficiency Benchmarking (NREL)
  - Hybrid Organic Inorganic Perovskite Synthesis (NREL)
- LBNL: Performing efficiency measurements, cell design and fabrication, and corrosion analysis.
  - Confirmed 100% faradaic efficiency
- NREL: Performing perovskite synthesis, on-sun testing, and cell reactor design
  - Design novel cell with dual-anode for accurate STH efficiency.







Collaboration enabled achievement of Solar-to-Hydrogen η = 20.8% and 102 hours of durability

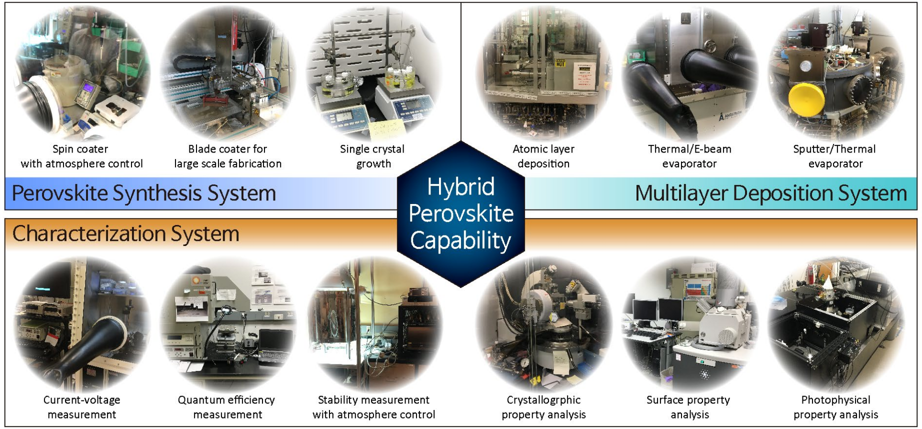
Deutsch, Toma, Mohite, et al. **2022**, submitted

Hybrid organic inorganic perovskite (HOIP) support

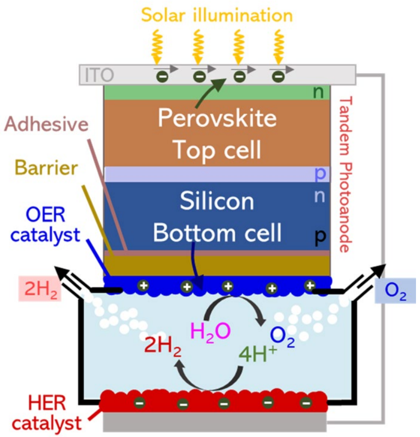
NREL HOIP capability supports several HydroGEN projects on PEC H_2 production, covering perovskite materials, devices, and characterizations:

- **Rice Univ:** (1) Co-planar all perovskites photocathode-photoanode device achieved STH ~13%, and lifetime ~23h; (2) Stacked perovskite/Si tandem device achieved STH ~20%, and lifetime ~100h (see schematics).
- **Univ of Toledo:** Stable perovskite/perovskite tandem electrodes for efficient PEC water splitting for H_2 production

Perovskite absorbers are promising for high-efficiency and low-cost PEC water splitting to produce hydrogen.

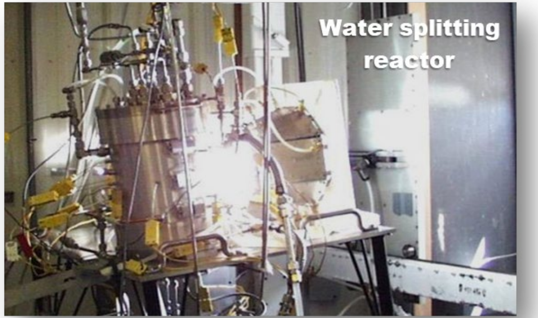


Schematics of unassisted PEC water-splitting system using HOIP/Si tandem (Aditya Mohite, Rice Univ)



NREL High Flux Solar Furnace (HFSF)

High Flux Solar Furnace | HydroGEN Consortium (h2awsm.org)



https://www.nrel.gov/csp/facility-hfsf.html
https://www.nrel.gov/news/features/2020/high-flux-solar-furnace.html

Purpose: NREL's HFSF is ideally suited for small-scale feasibility studies. It is available for on-sun functional component performance and materials testing for photo-electrochemical (PEC) cell and solar thermochemical (STCH) solar receiver.

Key Features:

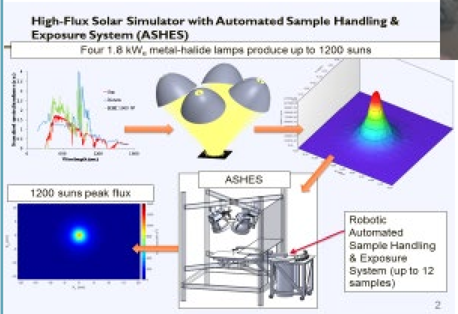
- NREL's HFSF consists of a tracking heliostat and 25 hexagonal slightly concave mirrors to concentrate solar radiation.
- The solar furnace can quickly generate over to 1,800°C over a 1-cm^2 area and up to 3,000°C with specialized secondary optics to generate concentrations greater than 20,000 suns.
- Flux levels and distributions can be tailored to the needs of a particular research activity.
- The operational characteristics and size of the facility make it ideal for testing over a wide range of technologies with a diverse set of experimental requirements.
- The facility can provide a platform for testing prototypes for solar-electric and solar-chemistry applications.

National Solar Thermal Test Facility (NSTTF)

National Solar Thermal Test Facility (NSTTF) | HydroGEN Consortium (h2awsm.org)

16kW
solar furnace

High-flux solar simulator

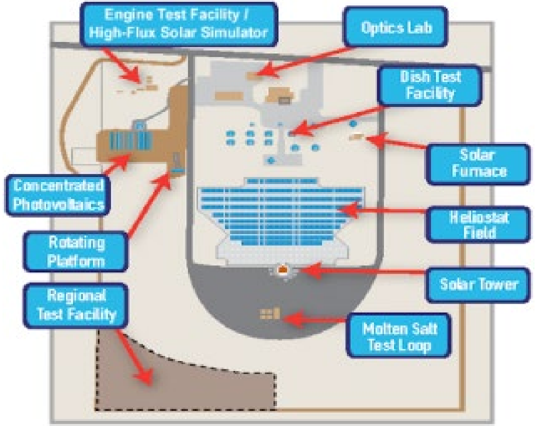


6 MW
power tower

http://energy.sandia.gov/energy/renewable-energy/solar-energy/csp-2/nsttf/

Key Features:

- Operated by Sandia National Laboratories for the U.S. Department of Energy (DOE), the National Solar Thermal Test Facility (NSTTF) is the only test facility of this type in the United States
- The NSTTF's primary goal is to provide experimental engineering data for the design, construction, and operation of unique components and systems in proposed solar thermal electrical plants planned for large-scale power generation.



Tips

- At proposal stage:
  - Go to HydroGEN capabilities website to search for lab capability
  - Email h2awsm@nrel.gov for capability suggestions and/or connect to capability experts
  - Engage with capability experts to better understand the capability and how to collaborate with them
    - e.g., modeling, synthesis, characterization, analysis
  - Work with the capability expert on the potential work scope to support the project
  - Choose 3-4 nodes to support your project to be most effective

Tips

- At awarded project stage:
  - Be ready to work with capability node experts at the beginning of project
  - Hold regular project team meetings with all so all have a big picture of the project & how each team member contributes to the work
  - Use the secure HydroGEN SharePoint project site to communicate with team members
    - share information: literature, background info, milestones
    - schedule meetings, take meeting notes
    - work on quarterly reports, AMR & conference presentations, and papers together
  - Share data in the secure HydroGEN Data Hub
    - Raw or processed data
    - Experimental & computational data
    - Synthesis & characterization data

Acknowledgements

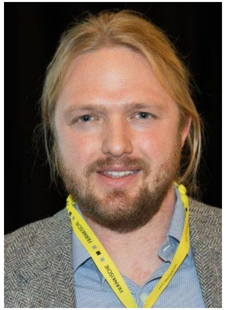
This work was fully supported by the U.S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy (EERE), Hydrogen and Fuel Cell Technologies Office (HFTO).

Ned Stetson

Katie Randolph

David Peterson

James Vickers



William Gibbons

Eric Miller

Interagency collaboration between NSF–DMREF projects and HFTO HydroGEN EMN
John Schlueter, Program Director, NSF–DMREF, Divisions of Materials Research

Questions?

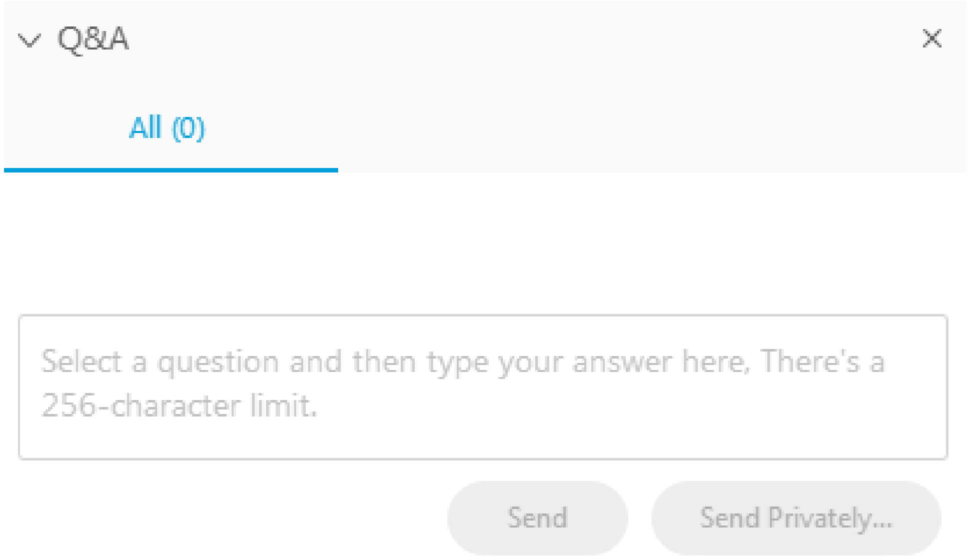
Email questions about HydroGEN capabilities to
h2awsm@nrel.gov

Email questions about FOA to
HFTOFOA@ee.doe.gov

INCREASE YOUR H2IQ hydrogen.energy.gov

The #H2IQ Hour Q&A

Please type your questions into the **Q&A Box**



INCREASE YOUR H_2IQ hydrogen.energy.gov

The #H2IQ Hour

Thank you for your participation!

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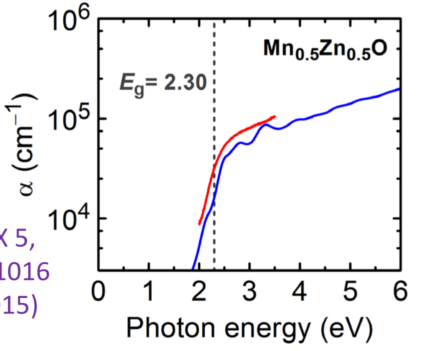
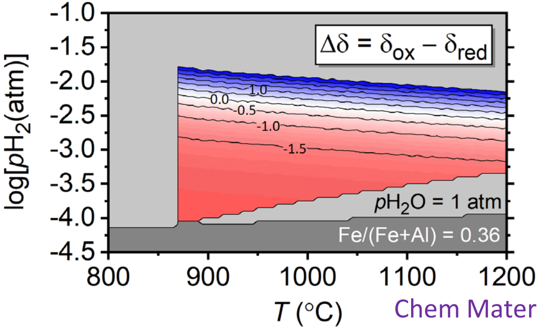
energy.gov/fuelcells
hydrogen.energy.gov

First Principles Materials Theory

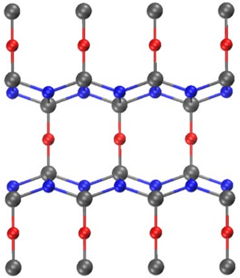
- Electronic structure prediction
  - Electronic structure prediction for transition metal oxides, complex large-scale systems (disorder, interfaces)
  - Band-structure, effective masses, density of states, ionization potential, band offsets, optical properties
- Defects and alloys
  - Advanced defect equilibria for non-dilute interacting defects, high-temperature redox processes, reduction entropies
  - Small-polaron transport vs band-like transport
  - Ionic diffusion pathways, energy barriers
  - Monte-Carlo simulations of disordered systems
- Materials Design and Discovery
  - Crystal structure predictions for bulk materials and interfaces
  - Convex hull analysis and phase diagrams



PRX 5, 021016 (2015)



Chem Mater 34, 519 (2022)

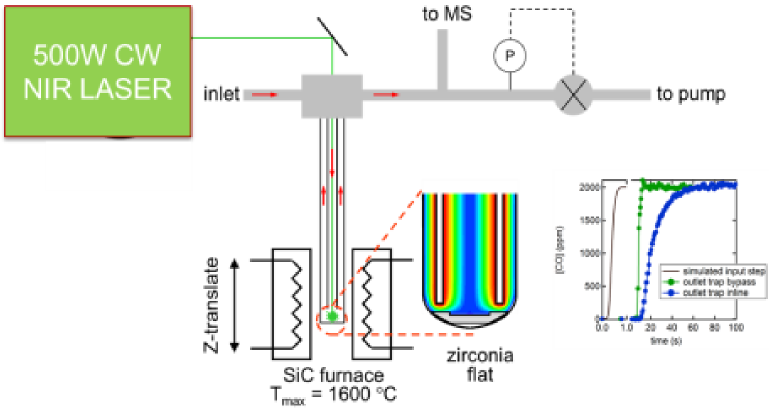


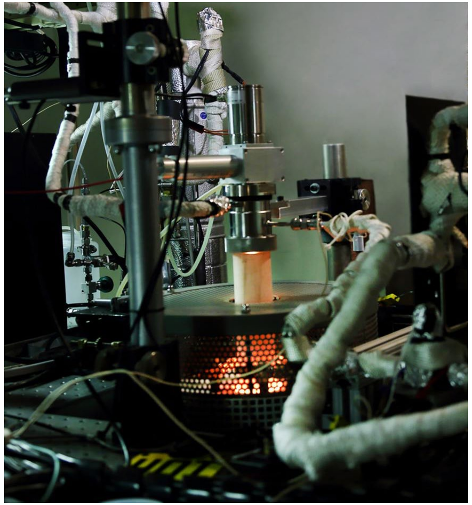
Ti_2ON_2 (sg 139)
E_g = 1.74 eV
m_e^* = 1.4 m_0
m_h^* = 4.7 m_0

JCP 154, 234706 (2021)

SNL Laser heated stagnation flow reactor for characterizing redox materials under extreme conditions

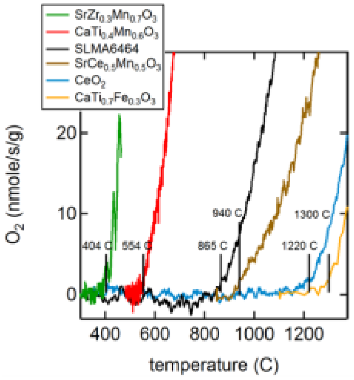
Measure reduction and oxidation rates under high radiative flux and rapid heating rates to <u>resolve detailed kinetics under extreme conditions</u>



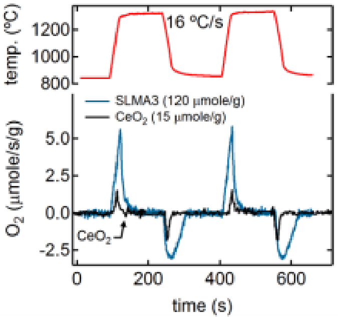


Laser-SFR reactor platform is <u>automated and virtually accessible</u> through remote windows desktop

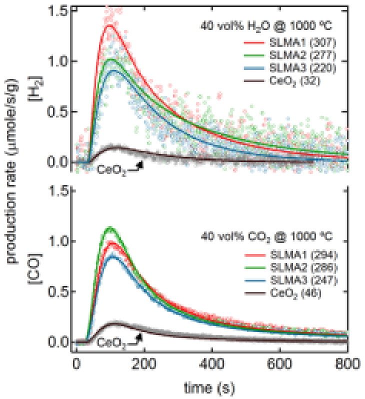
Temp. Prog. Red.



O_2 uptake/release



gas splitting



Benchmarking and Protocol Development for AWS Technologies

PI: Kathy Ayers, Proton OnSite (LTE)
Co-PIs: Ellen B. Stechel, ASU (STCH);
Olga Marina, PNNL (HTE);
CX Xiang, Caltech (PEC)
Consultant: Karl Gross

Goal: Development of best practices in materials characterization & benchmarking critical to accelerate materials discovery & development

Accomplishments:

- **3rd Annual AWS community-wide benchmarking workshop (ASU, Oct. 29–30, 2019)**
- **36 test protocols drafted and reviewed**
- **40 additional protocols in drafting process**
- **Relevant operational conditions were assessed for each of the water splitting technologies**
- **Engaged with new projects at March 2020 kickoff meeting and organized breakout meetings**
- **Quarterly newsletters disseminated to AWS community**

Development of best practices in materials characterization and benchmarking: critical to accelerate materials discovery and development

A Balanced AWSM R&D Portfolio

Low Temperature Electrolysis (LTE) (8 Projects)

- PEME component integration
- PGM-free OER catalyst
- Reinforced membranes

PEM Electrolysis

- PGM-free OER and HER catalyst
- Novel AEM and ionomers
- Bipolar membranes
- Electrodes

AEM Electrolysis

High Temperature Electrolysis (HTE) (8 Projects)

- Degradation mechanism at high current density operation
- Nickelate-based electrode and scalable, all-ceramic stack design
- Neodymium and lanthanum nickelate

O^{2-} conducting SOEC

- High performing and durable electrocatalysts
- Electrolyte and electrodes
- Low-cost electrolyte deposition
- Metal supported cells

H^{+} conducting SOEC

Photoelectrochemical (PEC) (7 Projects)

- III-V and Si-based semiconductors
- Chalcopyrites
- Thin-film/Si
- Protective catalyst system
- Tandem cell

Semiconductors

- PGM-free catalyst
- Earth abundant catalysts
- Layered 2D perovskites
- Tandem junction

Perovskites

Solar Thermochemical (STCH) (7 Projects)

- Computation-driven discovery and experimental demonstration of STCH materials
- Perovskites, metal oxides

STCH

- Solar driven sulfur-based process (HyS)
- Reactor catalyst material

Hybrid Thermochemical

PEME = proton exchange membrane electrolysis; AEME = alkaline exchange membrane electrolysis
PGM = platinum group metal; SOEC = solid oxide electrolysis cells