Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

HydroGEN Overview: A Consortium on Advanced Water Splitting Materials

H.N. Dinh, G. Groenewold, E. Fox, A. McDaniel, T. Ogitsu, A. Weber

Presenter: Huyen Dinh, NREL

Date: 5/20/2020

Venue: 2020 DOE Annual Merit Review

Project ID # P148

NREL | Berkeley Lab | Sandia National Laboratories | INL Idaho National Laboratory | Lawrence Livermore National Laboratory | SRNL

HydroGEN Overview

Timeline and Budget

- Start date (launch): **June 2016**
- FY17 DOE funding: **$3.5M**
- FY18 DOE funding: **$9.9M**
- FY19 DOE funding: **$8.4M**
- FY20 planned DOE funding: **$10.6M**
- Total DOE funding received to date: **$30M**

Barriers

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

Partners

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

BERKELEY LAB

Sandia National Laboratories

Lawrence Livermore National Laboratory

INL
Idaho National Laboratory

SRNL™

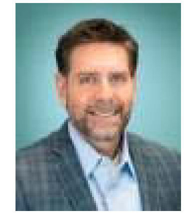
Collaboration: HydroGEN Steering Committee

NREL — NATIONAL RENEWABLE ENERGY LABORATORY

Huyen Dinh
(Director)

BERKELEY LAB

Adam Weber
(Deputy Director)



Sandia National Laboratories

Anthony McDaniel
(Deputy Director)

INL — Idaho National Laboratory

Richard Boardman

Lawrence Livermore National Laboratory

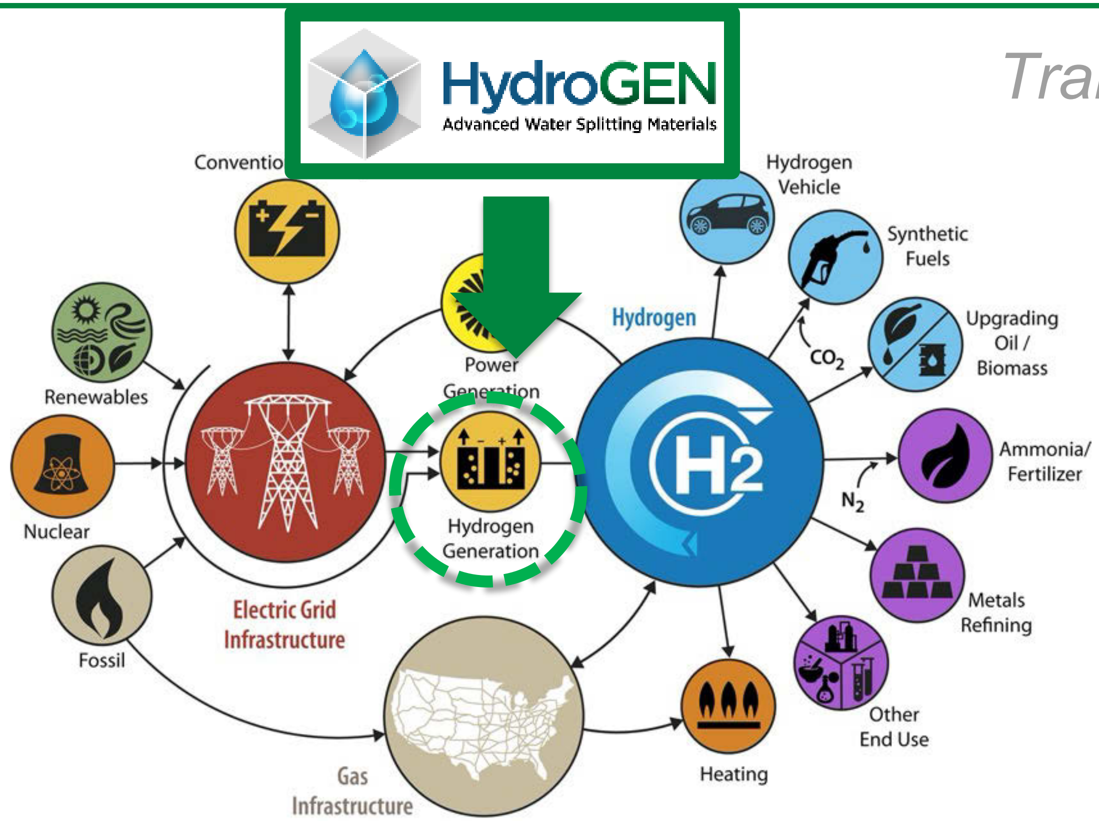
Tadashi Ogitsu

SRNL — SAVANNAH RIVER NATIONAL LABORATORY

Elise Fox

Ned Stetson and Katie Randolph, DOE-EERE-FCTO

H2@Scale Energy System Vision
Relevance and Impact



*Illustrative example, not comprehensive

Transportation and Beyond

Large-scale, low-cost hydrogen from diverse domestic resources enables an economically competitive and environmentally beneficial future energy system across sectors

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

https://energy.gov/eere/fuelcells/h2-scale

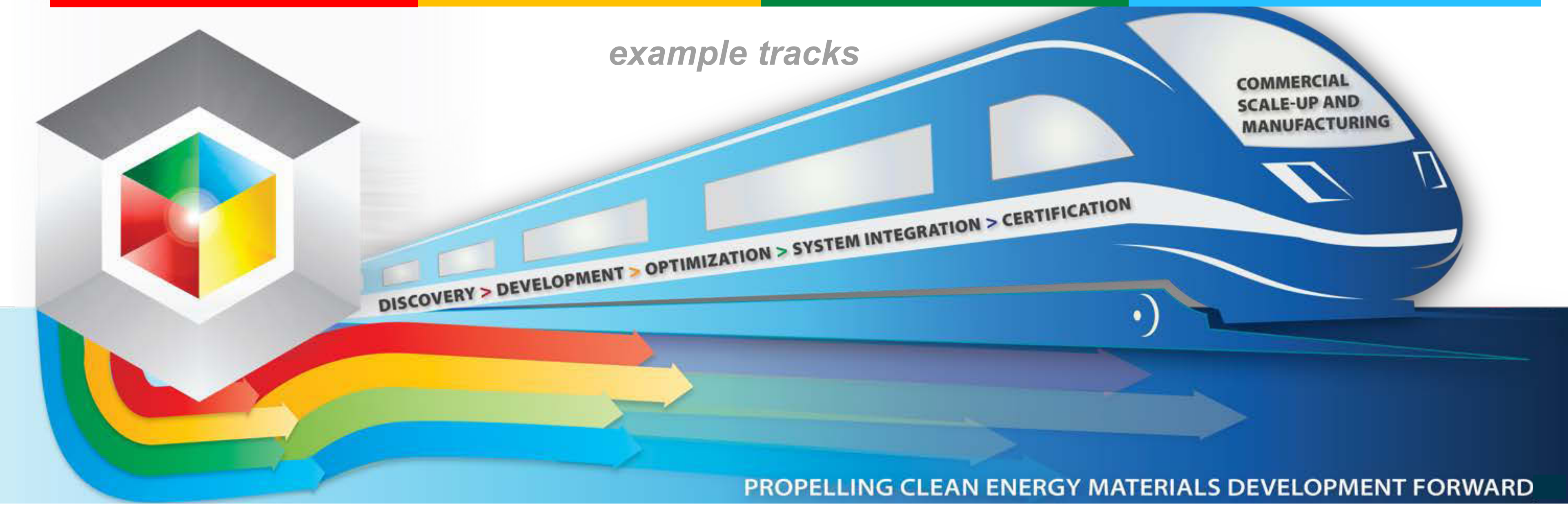
Hydrogen at Scale (H_2@Scale): Key to a Clean, Economic, and Sustainable Energy System, Bryan Pivovar, Neha Rustagi, Sunita Satyapal, *Electrochem. Soc. Interface* Spring 2018 27(1): 47-52; doi:10.1149/2.F04181if

Energy Materials Network (EMN)

Relevance and Impact

DOE's EMN aims to accelerate early-stage applied R&D in materials tracks aligned with some of the nation's most pressing sustainable energy challenges

Hydrogen Compatible Materials	Breakthrough Hydrogen Storage Materials	Advanced Water Splitting Materials for Hydrogen Production	Next-Generation Electro-catalysts for Fuel Cells



Accelerating early-stage materials R&D for energy applications

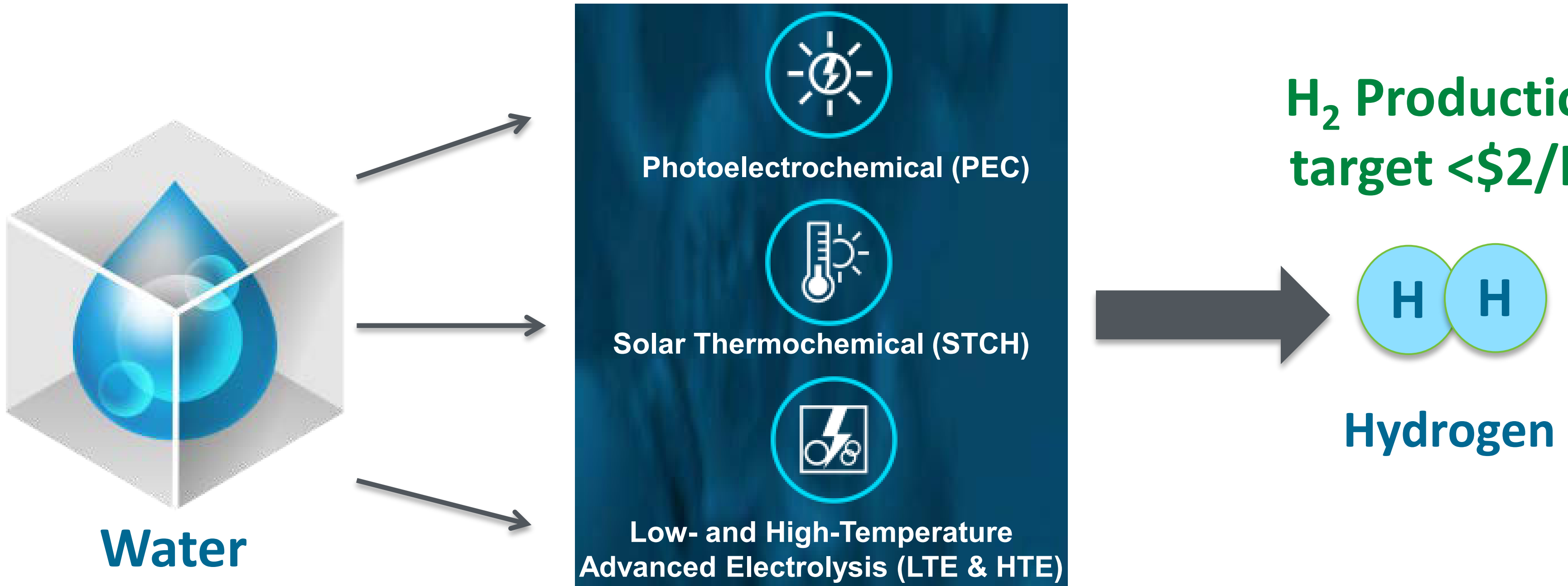
Advanced Water-Splitting Materials (AWSM)

Relevance, Overall Objective, Impact, and Approach

AWSM Consortium Six Core Labs:

NREL (National Renewable Energy Laboratory)
Berkeley Lab
Sandia National Laboratories
Idaho National Laboratory (INL)
Lawrence Livermore National Laboratory
SRNL

Accelerating R&D of innovative materials critical to advanced water splitting technologies for clean, sustainable, and low cost H_2 production, including:



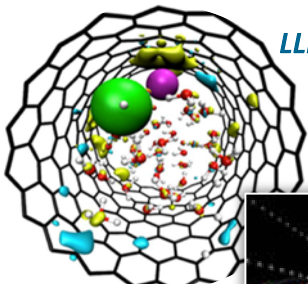
HydroGEN consortium supports early stage R&D in H_2 production

HydroGEN-AWSM Consortium

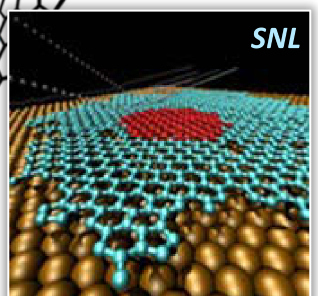
Relevance, Overall Objective, Impact, and Approach

Comprising more than 80 unique, world-class capabilities/expertise in:

Materials Theory/Computation

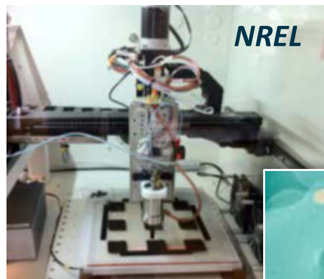


Bulk and interfacial models of aqueous electrolytes



LAMMPS classic molecular dynamics modeling relevant to H_2O splitting

Advanced Materials Synthesis

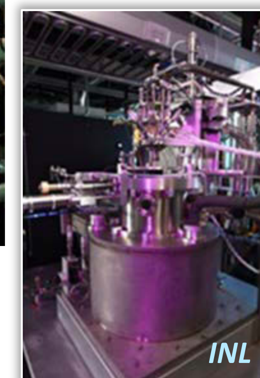


High-throughput spray system for electrode fabrication

Conformal ultrathin TiO_2 ALD coating on bulk nanoporous gold

Characterization & Analytics

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

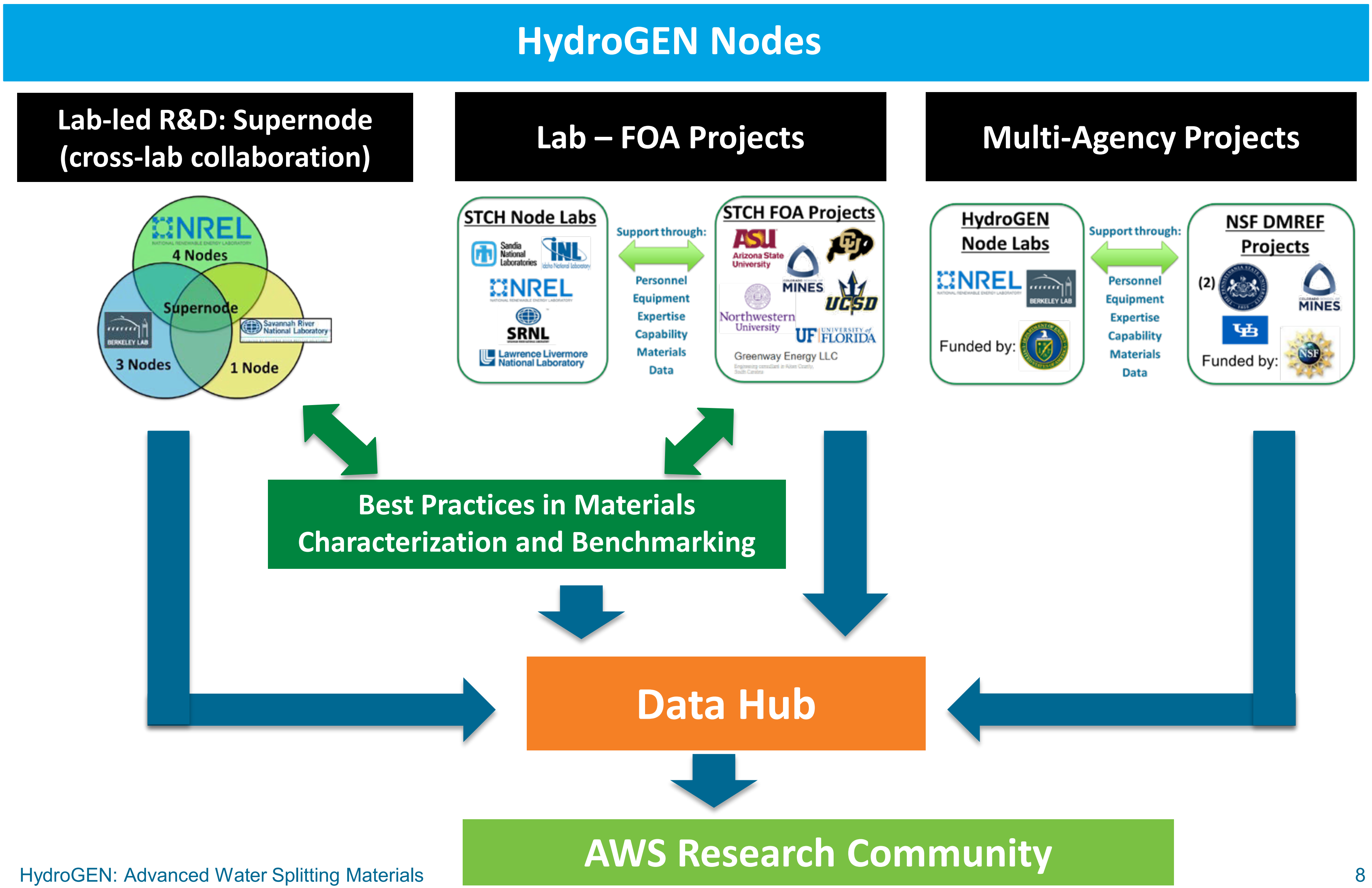


TAP reactor for extracting quantitative kinetic data

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/

Approach/Collaboration: HydroGEN EMN



Accomplishments: Developed New Publication Search Engine and Updated Capability Nodes

Developed **dynamic publications list** that pulls directly from **H2AWSM Zotero library**

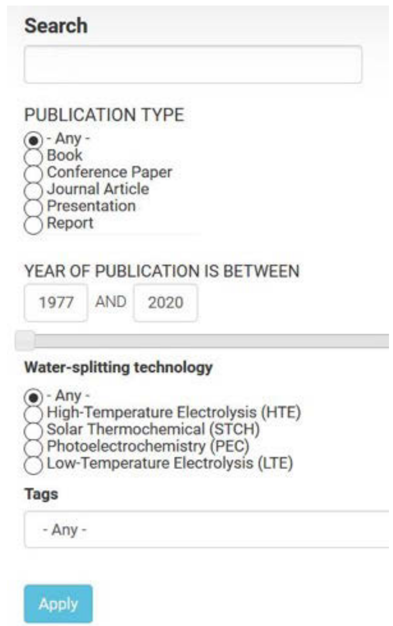
- Phase 1 (2020): HydroGEN publications and presentations
- Phase 2 (Future): All water-splitting literature resources

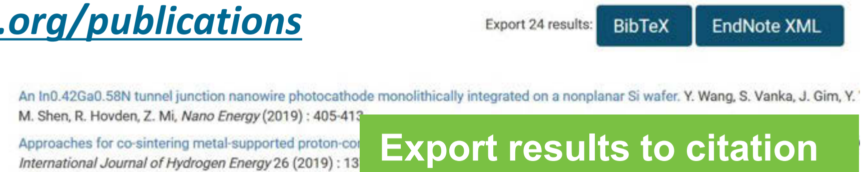
Added 1 new, updated >10 current, and **removed 2** capability nodes

- **New:** Microelectrode Testing of LTE Electrocatalysts, Ionomers, and Their Interactions in the Solid State

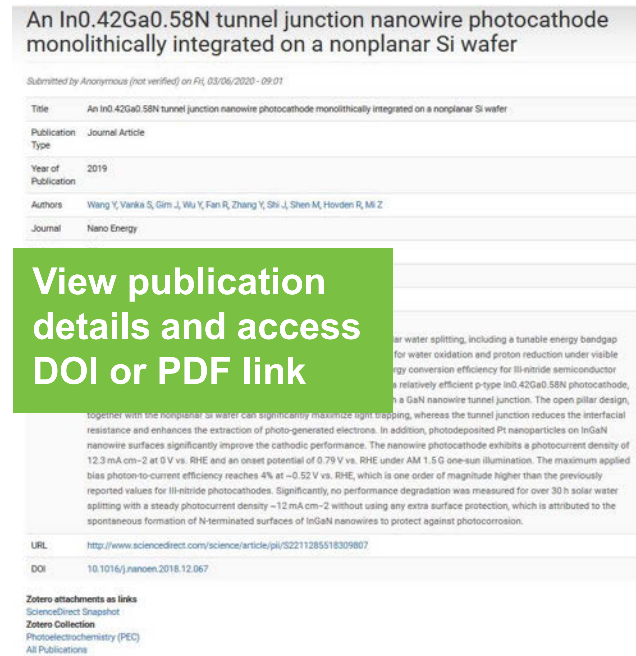
https://www.h2awsm.org/publications

Filter by type, year, AWS technology, and Zotero tags





Export results to citation management software



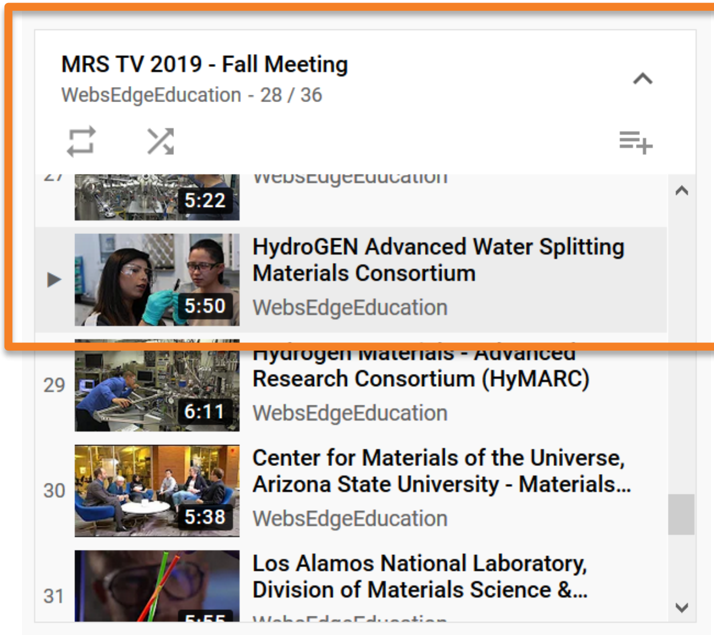
View publication details and access DOI or PDF link

Annual capability review is a rigorous process and keeps nodes updated and relevant

Accomplishments: Maintained HydroGEN Website and Participated in MRS TV Video

MRS TV Video

- Featured interviews and footage from across HydroGEN
- Broadcast at 2019 MRS Fall Meeting
- 3,137 views on MRS TV website
- Also posted on HydroGEN and DOE FCTO websites
- Raw footage can be used in additional consortium videos



Video can be found here:
https://youtu.be/PUti7ku2_ig

h2awsm.org →

5,407 users
7,353 sessions
23,382 pageviews

445 file downloads
629 video clicks

Traffic:
54% search
27% direct
18% referral

Top Pages:
Home
Capabilities

Accomplishments: HydroGEN Data Hub: Making Digital Data Accessible

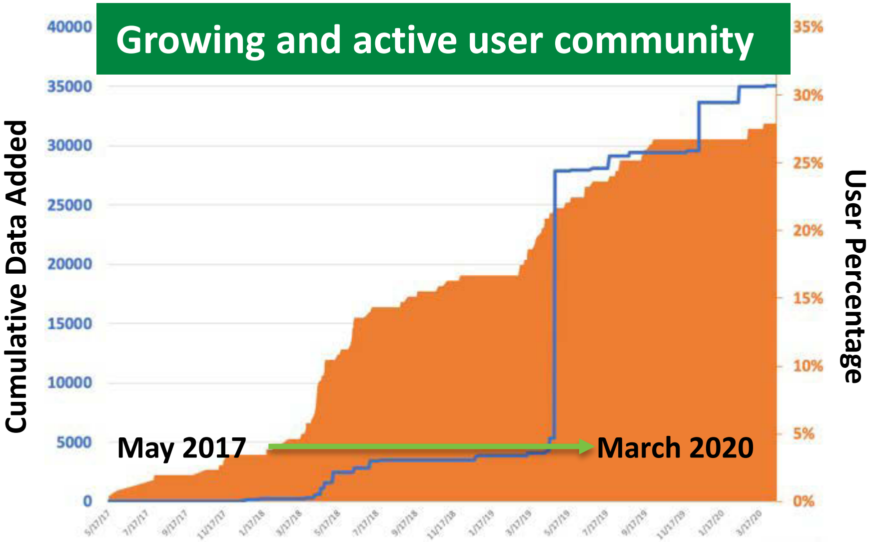
https://datahub.h2awsm.org/

User 179 → 258 (↑ 44%)

Files 4,055 → 36,580 (↑ 8000%)

Public Datasets: 21

Growing and active user community



Data Hub 2019-2020 Year in Review

- Grew Data Hub community and site visits
- Implemented data governance processes
- Upgraded Data Hub software platform
- Expanded visualization of multi-spectra data
- Developed metadata for each AWS technology
- Metadata endpoints – data curation, improved upload.

Many Types of Experimental Data

Material characterization

- XRD, SFR, XPS, XRF, SEM, TEM, Raman,

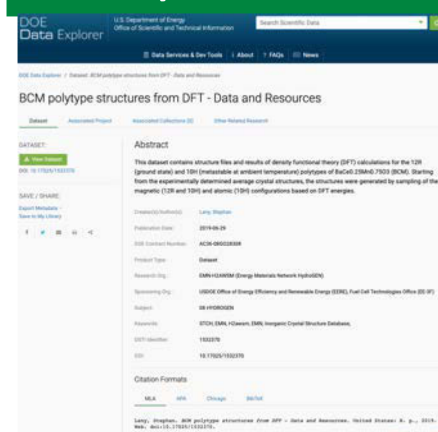
Device performance

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

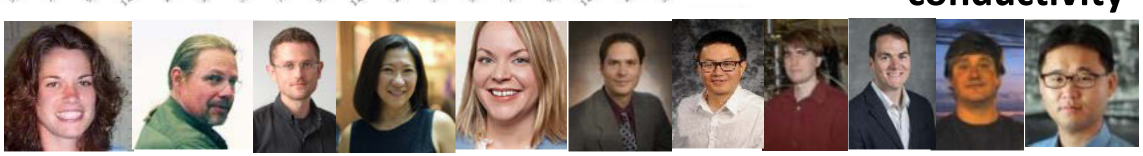
Materials durability data

- TGA, membrane conductivity

Assigning a Digital Object Identifier (DOI) to public datasets for a persistent landing page and scientific discovery.



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



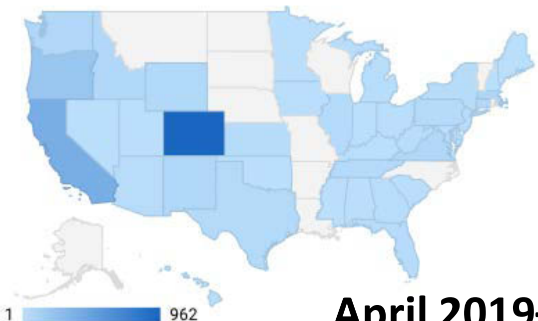
Data Team

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

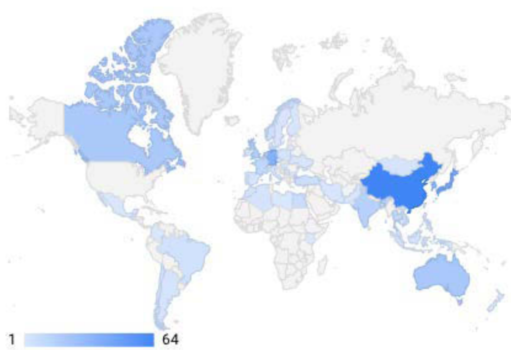
Accomplishments:
Data Hub Metrics and Data Governance

Data Hub Metrics: Tracking Access and Utilization

- 414 Data Hub visits from outside the United States
- 2,387 visits from within the United States
- 786 sessions are from users logging in to contribute to private data within projects.



April 2019–April 2020



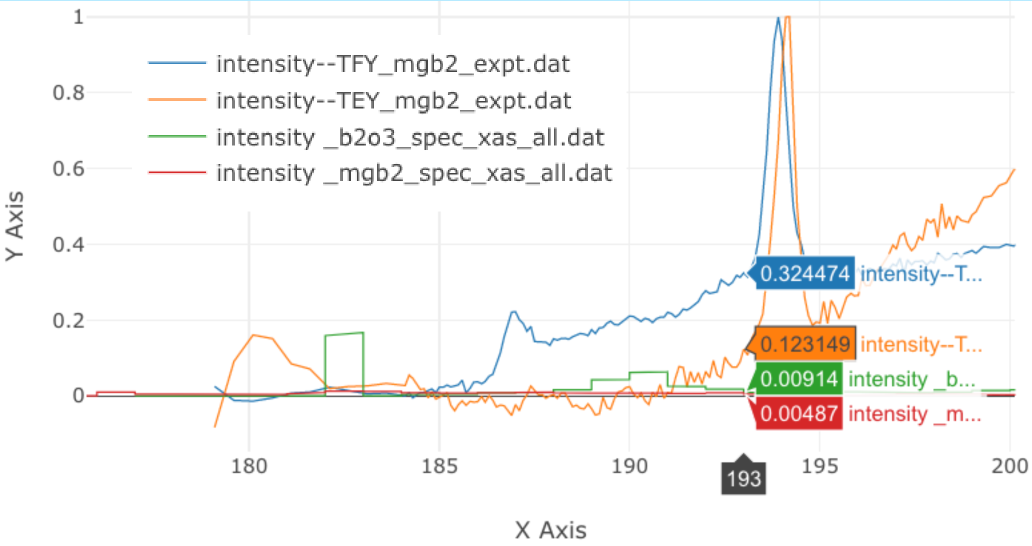
Data Governance for Availability, Usability, Integrity and Security

New User Resources include:

- Metadata API endpoints
- Updated data release procedure
- Project closeout procedure
- Zotero tutorial
- Terms and privacy policy

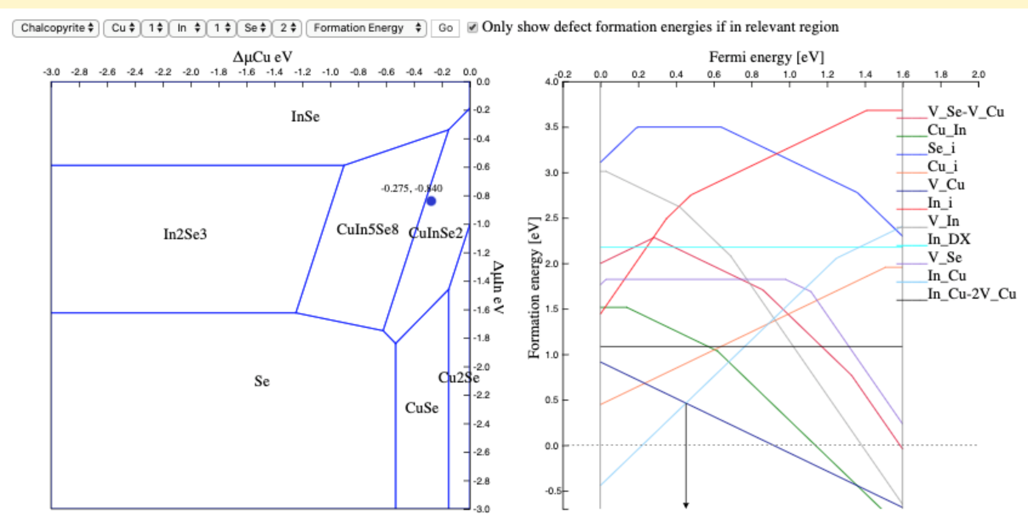
- FAIR data standard
- Better data quality and usability
- Increased availability and accessibility

Accomplishments: Data Tools for Visualization and Analysis: Multi-Spectra and Phase and Defect Formation Diagram



The interactive **Advanced Multi-Spectra Data View** allows many spectra files (any csv or tabular file format) to be visualized at one time, from one or many files.

https://bit.ly/2Vss96E



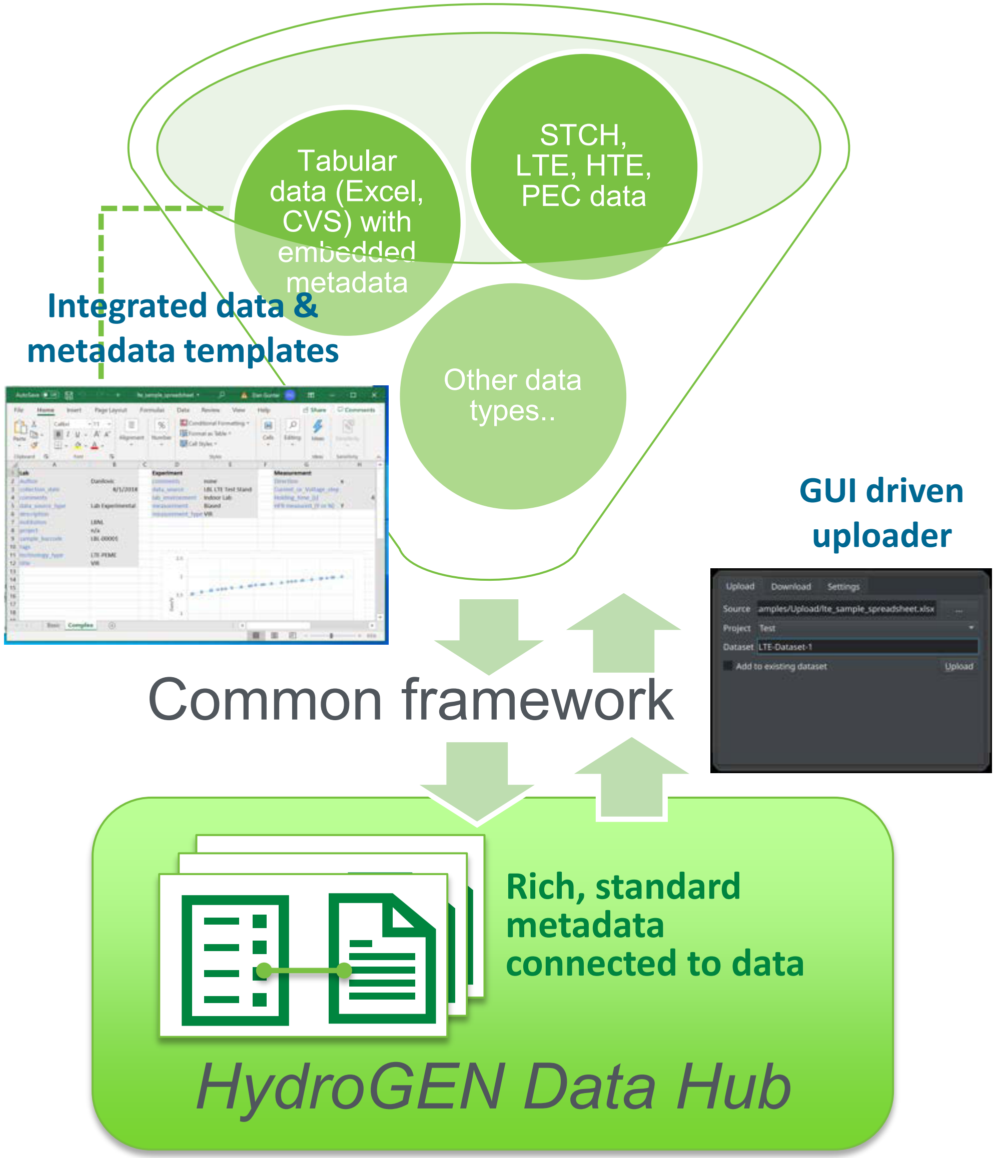
LLNL developed the dynamic GUI for **Defect Analysis** that generates the defect stability plot (right) for a given alloy composition (left: click a point in alloy phase diagram), and NREL implemented it on the Data Hub for photoabsorber (PEC) and STCH materials development.

https://bit.ly/3aoGVjb

Accomplishments: Metadata Automation and Standardization

Metadata is crucial to efficient utilization of stored data

- Capture all information about source, experiment, computation, sample, measurement, and result
  - Enable powerful searching across datasets
- Automate metadata capture and upload/download tasks
  - Standard templates
  - GUI-based framework
  - User-friendly and error-free
- Python parsing architecture facilitates customization
- Shared code in Github facilitates collaboration



Accomplishments: Technology Transfer Agreements (TT/A)

➢ Streamlined Access

- ✓ **Four** standard, pre-approved TT/A between all consortium partners
  - ✓ Non-Disclosure Agreement (NDA)
  - ✓ Intellectual Property Management Plan (IPMP)
  - ✓ Materials Transfer Agreement (MTA)
  - ✓ Cooperative Research and Development Agreement (CRADA)
- ✓ Updated NDA
- ✓ Executed all 33 project NDAs

Non-Disclosure Agreement (NDA) → Information Disclosure

Intellectual Property Management Plan (IPMP) → IP Protection

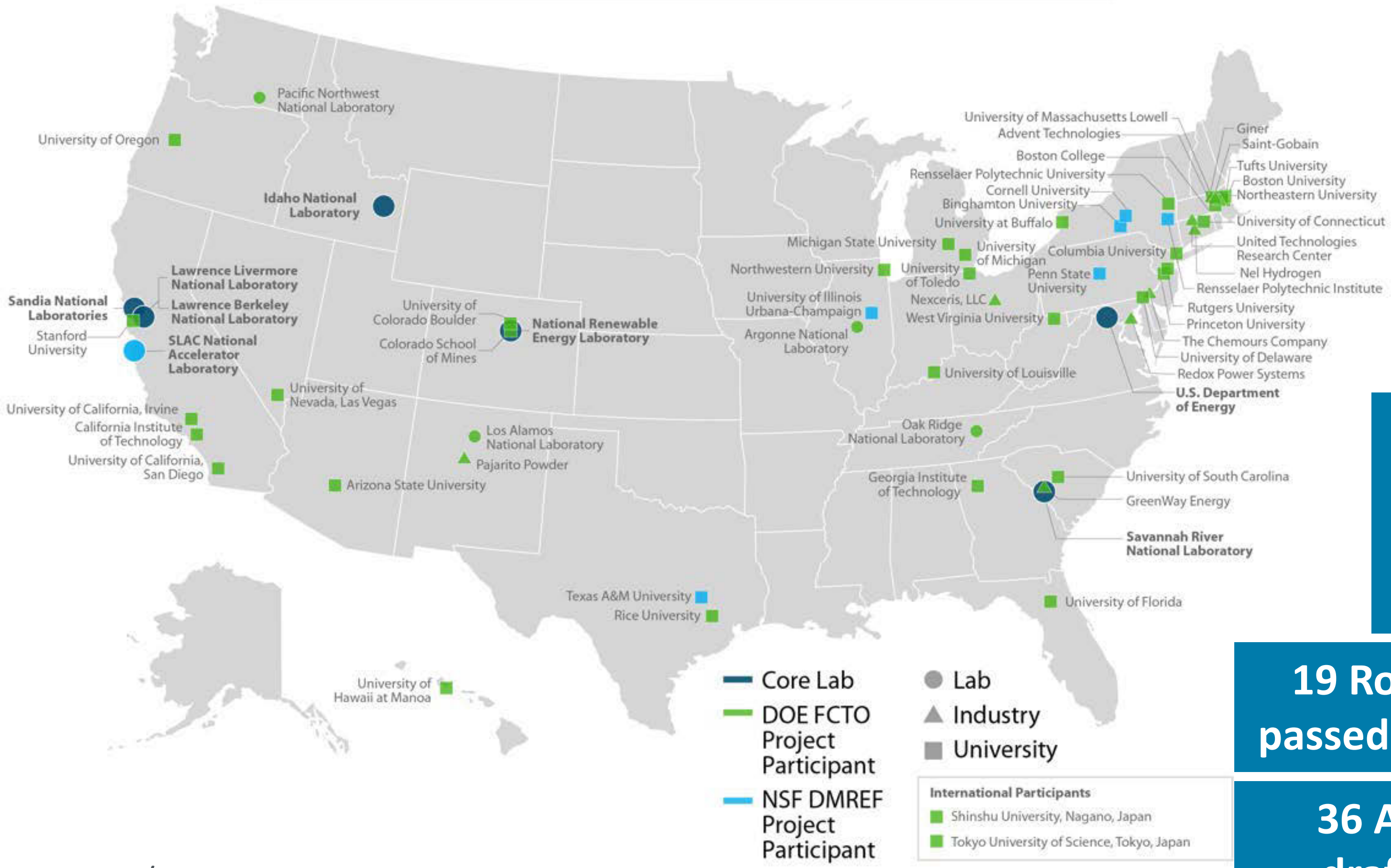
Materials Transfer Agreement (MTA) → Freedom to Operate

Cooperative Research and Development Agreement (CRADA) → Collaboration

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

National Innovation Ecosystem
Collaboration/Accomplishments

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



GNG: Go/No-Go

2 Community Benchmarking Workshops

11 new Round 2 FOA projects

5 Supernodes passed GNG

4 Interagency (NSF DMREF – DOE EERE HFTO EMN) projects completed

19 Round 1 FOA projects passed GNGs and in phase 3

36 AWS test protocols drafted and reviewed

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

NSF DMREF PSU LTE (Interagency Collaboration/Accomplishments)

Membrane Databases – New Schema and Dissemination

Membrane Databases – New Schema and Dissemination

(Supplement to: Development of Design Rules for High Hydroxide Transport in Polymer Architectures)

Michael Hickner
Penn State

Chulsung Bae
RPI

Stephen Paddison
UT Knoxville

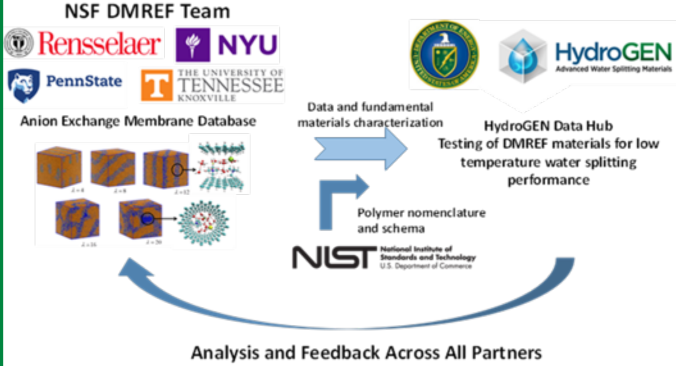
Mark Tuckerman
NYU

Debra Audus
NIST

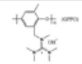
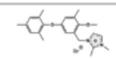
Kristin Munch
NREL

Huyen Dinh
NREL

Membrane Databases New Schema and Dissemination



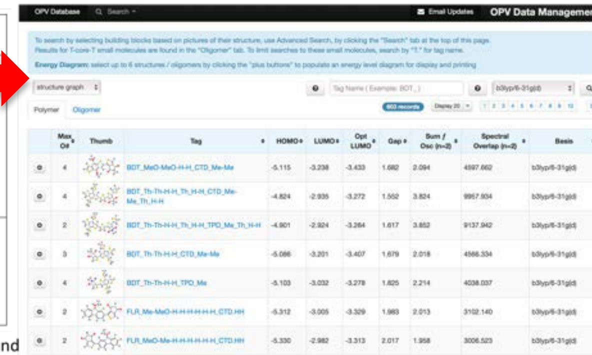
NSF DMREF Project Membrane Database

	Cation Structure	Backbone Structure	IEC (mmol/g)	Anion conductivity (mS/cm)	Swelling ratio (%)	Water uptake (%)	Alkaline stability	Ref
1.		PPO	2.69	71 (25°C)	12.5 (25°C) 18.9 (80°C)	49.9 (25°C) 72.9 (80°C)		1
2.			2.23	64 (25°C)	25.0 (25°C) 45.0 (80°C)	77.1 (25°C) 98.7 (80°C)	1M KOH @ 25°C, 8 days, no degradation	
3.	BTMA		2.65	44 (25°C)	37.5 (25°C) 75.6 (80°C)	100.6 (25°C) 430.1 (80°C)	20-40% loss of QA (come from other refs)	
4.	 (DMI)		2.8	40 (25°C) 75 (60°C)	37.5 (20°C)	136.7 (20°C)		2
5.			2.5	35 (25°C) 65 (60°C)	30.3 (20°C)	102.2 (20°C)	2M KOH @ 25°C, 9days, No degradation 2M KOH @ 60°C, 9days, Loss of IEC=50%	

Will also scope automated machine reading of the literature - see Olivetti, et al.

...65 and counting

Where We Want To Go



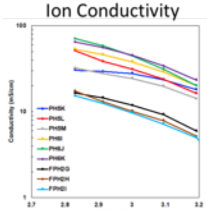
https://organicelectronics.nrel.gov/project/detail/project_id/19

HydroGEN capabilities and expertise

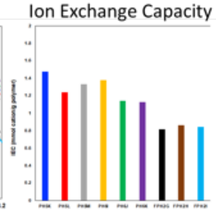
NREL's AEM Polymer Library

Bryan Pivovar
Kelly Meek

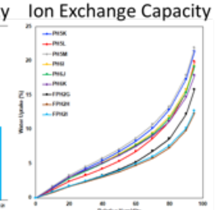
Ion Conductivity



Ion Exchange Capacity

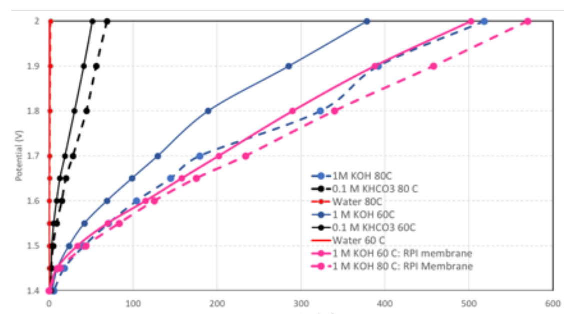


Ion Exchange Capacity



NREL Electrolyzer Testing

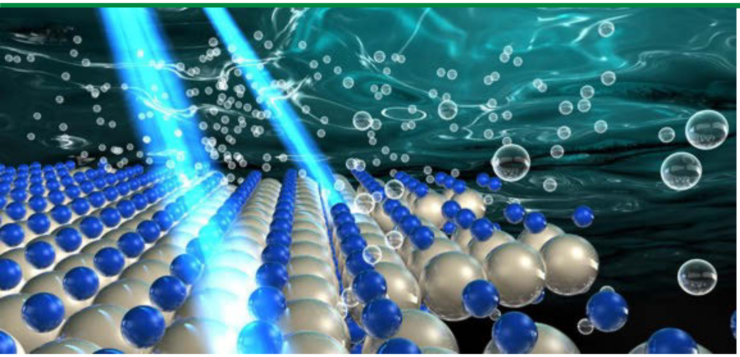
Guido Bender
Shraboni Ghoshal



Interagency collaboration enables development of an integrated membrane database with new schema and dissemination

NSF DMREF UB PEC (Interagency Collaboration/Accomplishments)

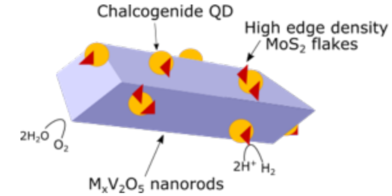
A Blueprint for Photocatalytic Water Splitting: Mapping Multidimensional Compositional Space to Simultaneously Optimize Thermodynamics and Kinetics



DMREF – HydroGEN Collaboration

Goal: Accelerate Pt-free ternary photocatalysts $M_xV_2O_5/CdX/MoS_2$ for solar hydrogen generation

Collaboration Achievements: Integrating MoS_2 co-catalysts to rationally designed photocatalysts

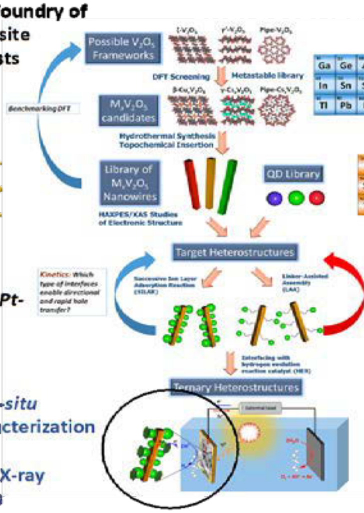


A. Parija et al., *ACS Cent. Sci.* **2018**, 4, 4, 493-503

Banerjee, Watson, Piper, to be submitted

Collaboration: Material Discovery & Advanced

1. Increase Foundry of Nanocomposite Photocatalysts



2. Develop Pt-free co-catalysts

3. Adapt In-situ X-ray Characterization

4. Perform X-ray simulations

Sarbajit Banerjee (Texas A&M)

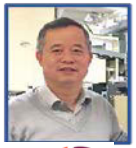
David Watson (Buffalo)

Louis Piper (Binghamton)

Jinghua Guo

David Prendergast

(LBNL)

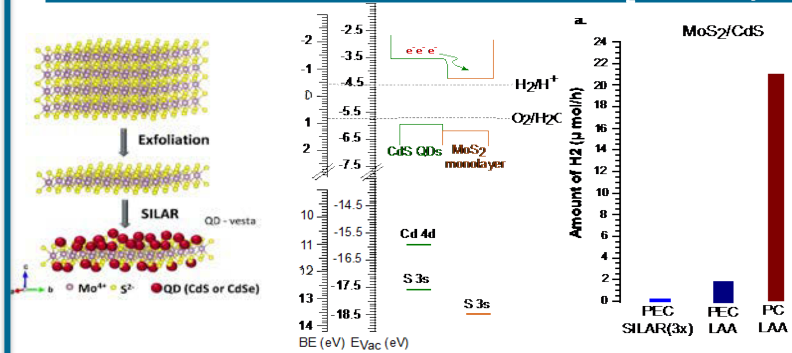


HydroGEN Advanced Water Splitting Materials

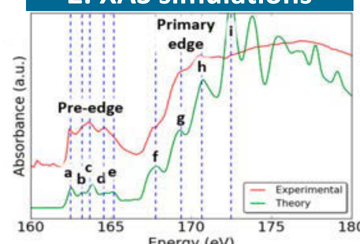
BERKELEY LAB MOLECULAR FOUNDRY

ALS

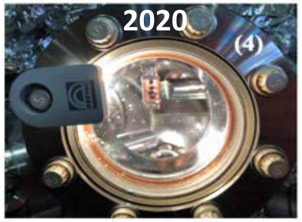
1. Confirmed suitable band offsets of MoS_2 co-catalyst



2. XAS simulations



3. *Operando* XAS – March 2020



Leveraging HydroGEN advanced characterization and modeling enabled deeper understanding of photocatalysts for solar hydrogen generation; accelerating the design of novel third-generation ternary heterostructured catalysts

NSF DMREF PSU PEC (Interagency Collaboration/Accomplishments)

Experimental Validation of Designed Photocatalysts For Solar Water Splitting

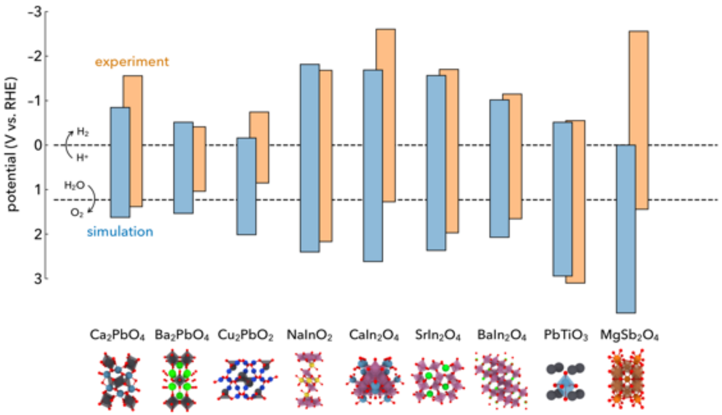
Catherine Badding,[1] Ismaila Dabo,[2] Raymond E. Schaak,[3] Héctor D. Abruña[1]
[1]Chemistry and Chemical Biology, Cornell, [2]Materials Science, Penn State, [3]Chemistry, Penn State

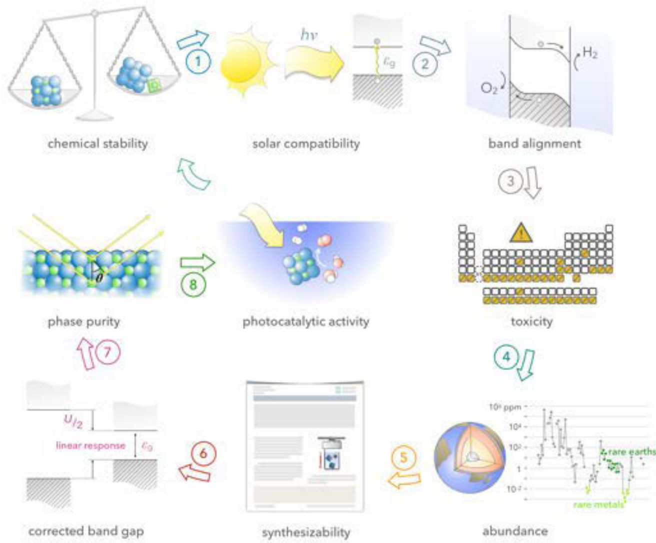
National Foundation,
Award No. Science DMREF/INFEWS-1729338

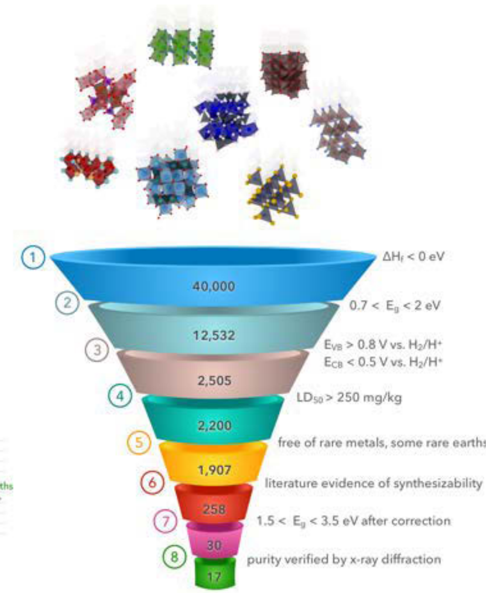
Cathy Badding
DOE *SULI Awardee* (2018)
Goldwater Scholar (2019)

Dropped-casted films from synthesized powders

Experiments confirm favorable redox alignment and hydrogen generation for 9 of the 14 synthesized compounds, with the most promising ones belonging to the families of alkali and alkaline-earth indates and plumbates.







NATIONAL RENEWABLE ENERGY LABORATORY

HydroGEN Advanced Water Splitting Materials

Collaboration enabled development of a screening procedure (with co-validation between experiment and theory) to expedite the synthesis, characterization, and testing of the computationally predicted, most attractive materials.

High Temperature Defects: Linking Solar Thermochemical and Thermoelectric Materials

High Temperature Defects: Linking Solar Thermochemical and Thermoelectric Materials

NSF-DMREF: Prashun Gorai, Vladan Stevanovic, Eric Toberer
Colorado School of Mines, Golden, CO 80401

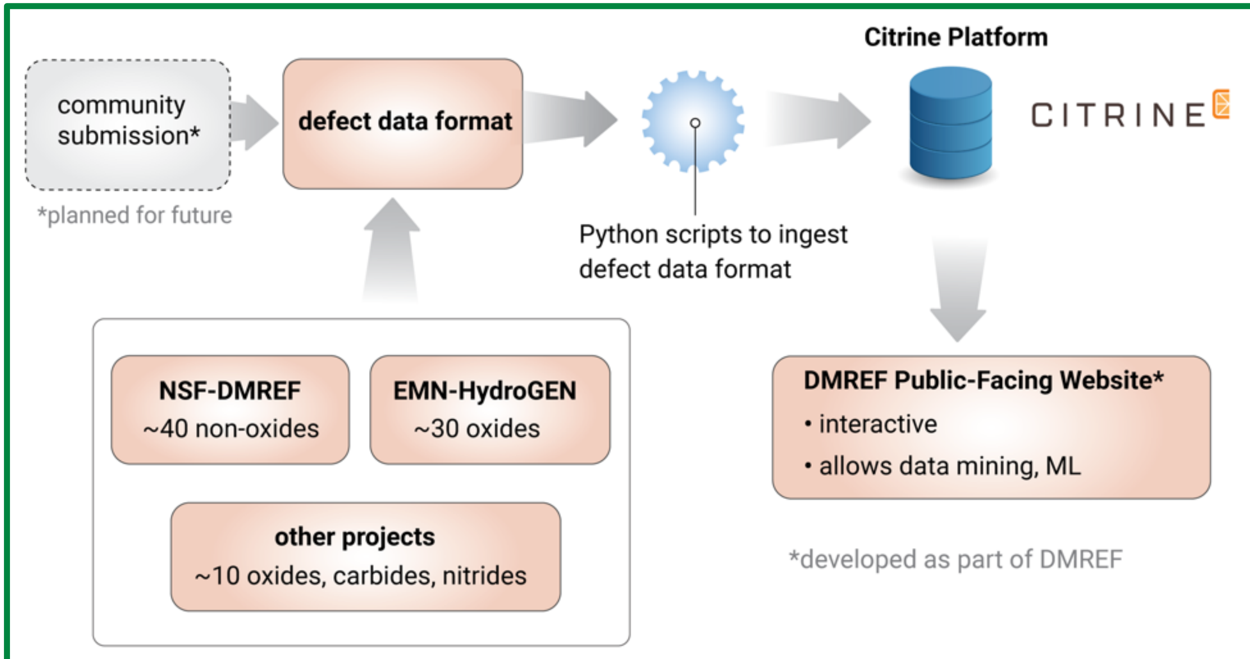
DOE-EMN: Jie Pan, Stephan Lany
National Renewable Energy Laboratory, Golden, CO 80401

External Collaborator: Chris Borg
Citrine Informatics, Redwood City, CA 94063

Designing Materials to Revolutionize and Engineer our Future (DMREF)

Energy Materials Network
U.S. Department of Energy

Collaboration Goal: Leverage non-oxide (DMREF) and oxide (HydroGEN EMN) defect calculations to build a comprehensive database of defect calculations.



***Impact**: Creation of a central repository of defect calculations that will allow data informatics approaches for predicting dopability.*

***Lessons**: To build reliable machine learning (ML) models, need for diverse (composition, structure) dataset; possible by leveraging multiple projects.*

Collaboration: HydroGEN FOA-Awarded Projects

31 FOA-Awarded Projects

43 unique capabilities being utilized across six core labs

Advanced Electrolysis (16)	PEC (7)	STCH (7)
LTE (8) HTE (8)	Benchmarking & Protocols (1)	2-Step MO_x(6) Hybrid Cycle (1)

A Balanced AWSM R&D Portfolio

Approach/Collaboration

Low Temperature Electrolysis (LTE)
(G. Bender: P148C; 8 Projects)

PEME Component Integration

- PGM-free OER and HER catalyst
- Novel AEM and Ionomers
- Electrodes

PEM Electrolysis

nel
Argonne NATIONAL LABORATORY
Chemours

AEM Electrolysis

Northeastern University
Center for Renewable Energy Technology
Los Alamos NATIONAL LABORATORY (2)
Georgia Institute of Technology
UNIVERSITY OF OREGON

High Temperature Electrolysis (HTE)
(G. Groenewold: P148D; 8 Projects)

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

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

O^{2-} conducting SOEC

NEXCERIS where energy meets environment
REDOX Redox Power Systems, LLC
Northwestern University
SAINT-GOBAIN

H^+ conducting SOEC

United Technologies Research Center
West Virginia University
UNIVERSITY OF South Carolina
University of Connecticut

Photoelectrochemical (PEC)
(N. Danilovic: P148A; 7 Projects)

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

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

Semiconductors

STANFORD UNIVERSITY
University of Hawaii
THE STATE UNIVERSITY OF NEW JERSEY RUTGERS

Perovskites

UNIVERSITY OF MICHIGAN
University of California, Irvine
RICE
THE UNIVERSITY OF TOLEDO

Solar Thermochemical (STCH)
(A. McDaniel: P148B; 7 Projects)

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

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

STCH

ASU Arizona State University
COLORADO SCHOOL OF MINES
University of Colorado
UCSD

Hybrid Thermochemical

Northwestern University
Greenway Energy LLC
Engineering consultant in Aiken County, South Carolina
UF UNIVERSITY of FLORIDA

PEME = proton exchange membrane electrolysis;
AEME = alkaline exchange membrane electrolysis

PGM = platinum group metal
Solid oxide electrolysis cells: SOEC

Collaboration: Top HydroGEN Capability Nodes By Project Utilization (LTE, HTE, PEC, STCH projects)

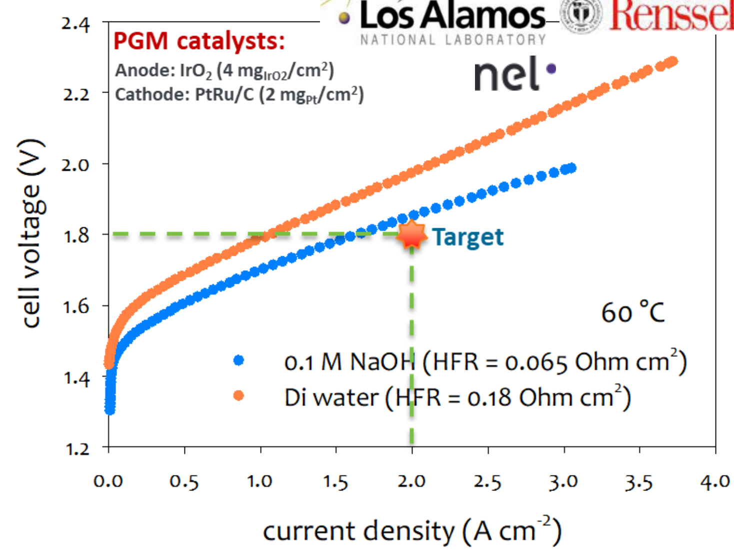
HydroGEN Capability Node	Node Class	LTE	HTE	PEC	STCH
LBNL Multiscale Modeling of Water Splitting Devices	Modeling	9			
INL Advanced Materials for Elevated Temperature Water Electrolysis	Characterization		9		
NREL In-Situ Testing Capabilities for Hydrogen Generation	Characterization	8			
NREL Thin Film Combinatorial Capabilities for Advanced Water Splitting Technologies	Synthesis + Characterization		3	2	2
NREL First Principles Materials Theory for Advanced Water Splitting Pathways	Modeling				6
NREL On-Sun PEC Solar-to-Hydrogen Benchmarking	Characterization			6	
LBNL Thin Film and Bulk Ionomer Characterization	Characterization	6			
SNL High-Temperature X-ray Diffraction and Thermal Analysis	Characterization		1		5
NREL Multi-Component Ink Development, High Throughput Fabrication, and Scaling Studies	Processing & Scale Up	5			
SNL Virtually Accessible Laser Heated Stagnation Flow Reactor	Characterization				5
LLNL Ab Initio Modeling of Electrochemical Interfaces	Modeling			4	1

HydroGEN characterization capability nodes are the most utilized by projects across different AWS technologies

Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

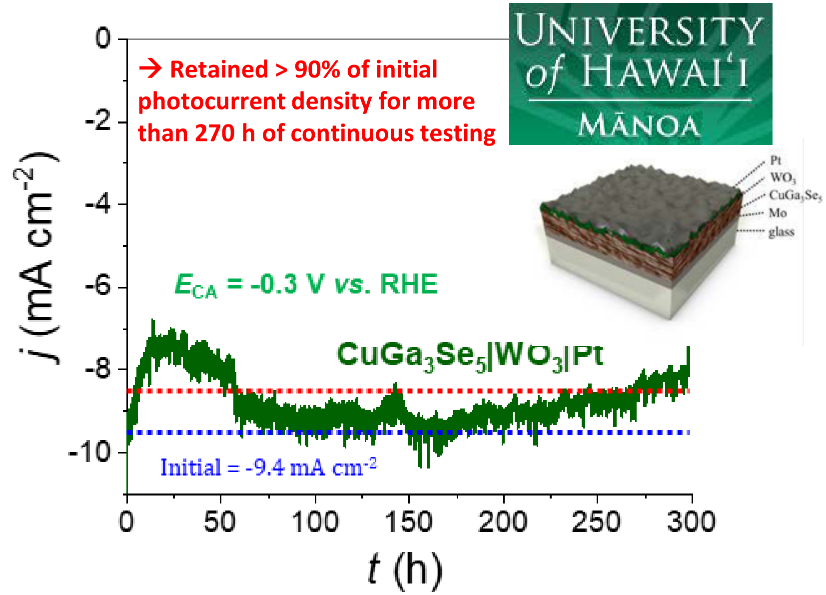
Low Temperature Electrolysis (LTE)

LANL, Rensselaer Polytechnic Institute, and Nel demonstrated **high AEM electrolyzer performance that approaches the 2020 target (2 A/cm^2 at 1.8 V, 60°C)** using polystyrene based alkaline polymers that are durable and economically affordable. SNL provided control AEM and ionomer and NREL nodes studied the effect of pH on AEM performance. LBNL modeling and characterization nodes helped LANL better understand the ionomer stability, ionomer/catalyst interface, and pH effect.



Photoelectrochemical (PEC) Water Splitting

University of Hawaii **extended chalcopyrites durability to 270 hours** using atomic layer deposition (ALD) WO_3 coatings, paving the way to creating a low cost ("printed") chalcopyrite-based, semi-monolithic, tandem hybrid photoelectrode device prototype that can operate for at least 1,000 h with solar-to-hydrogen efficiency >10%. This project is supported by NREL synthesis and advanced characterization and LLNL modeling expertise to accelerate the development of materials and interfaces.

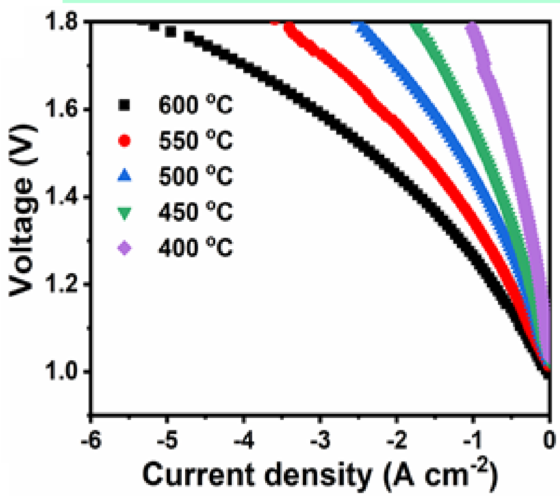


Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

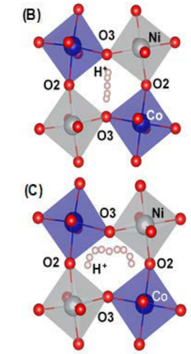
High Temperature Electrolysis (HTE)

University of Connecticut, with INL, successfully developed a new triple-phase conducting oxide, PNC perovskite, as an oxygen electrode in **proton conducting solid oxide electrolysis cells (H-SOEC)**, exhibiting good electrochemical performance at reduced temperatures of 400°–600°C. **The electrolysis current density achieved (1.72 A/cm^2 at 1.4 V and 600°C) is the highest performance to date.** Furthermore, H-SOECs with this electrode material showed robust durability for thermal cycling and reversible operation at these temperatures.

Best SOEC performance



University of Connecticut

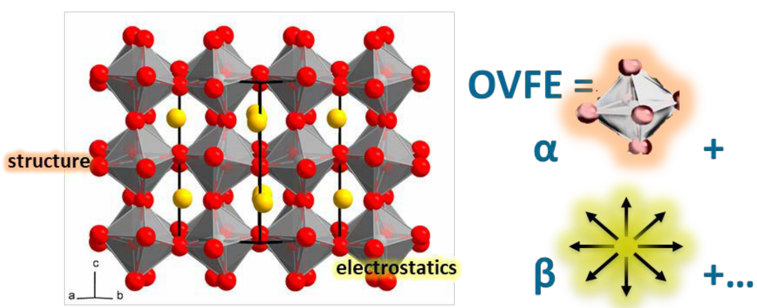


Solar Thermochemical (STCH) Water Splitting

Arizona State University (ASU) and Princeton computationally predicted, and NREL synthesized, **a ternary oxide STCH material for water splitting that has the potential to achieve higher specific capacities and larger H_2 to H_2O ratios and meet the hydrogen production cost targets.** These results point to the importance of both valence state and crystalline structure in achieving large degrees of reversible reduction and open the door to a new class of STCH materials.

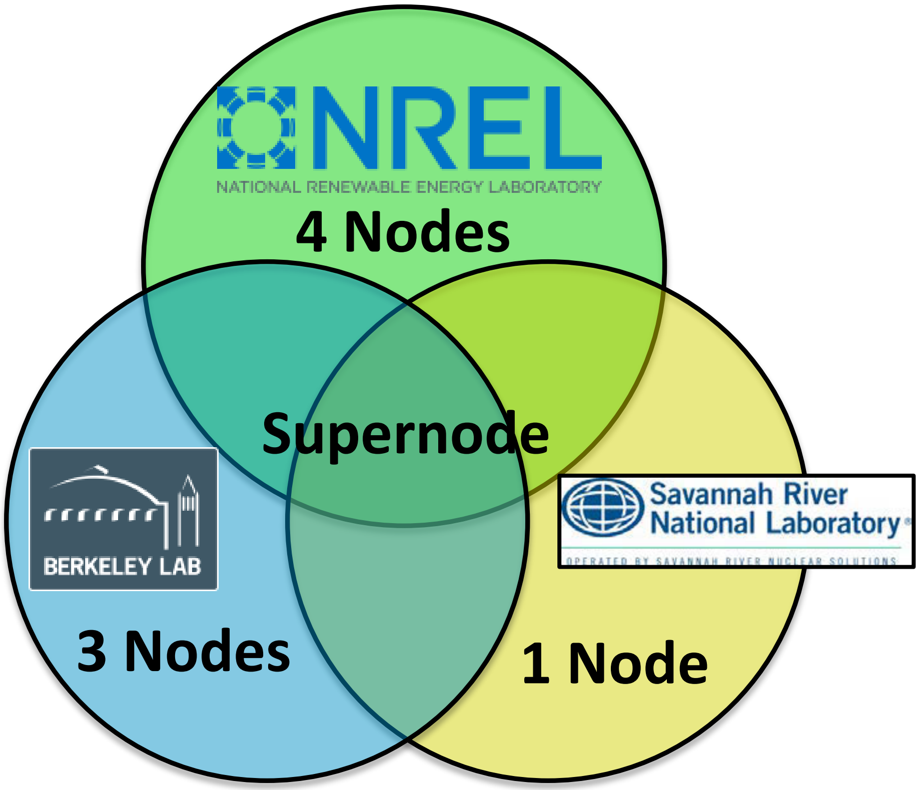
ASU

Materials design principles from machine learning



Five New Supernodes: Accelerate AWSM Materials R&D through Lab Collaboration

LTE Supernode (example)

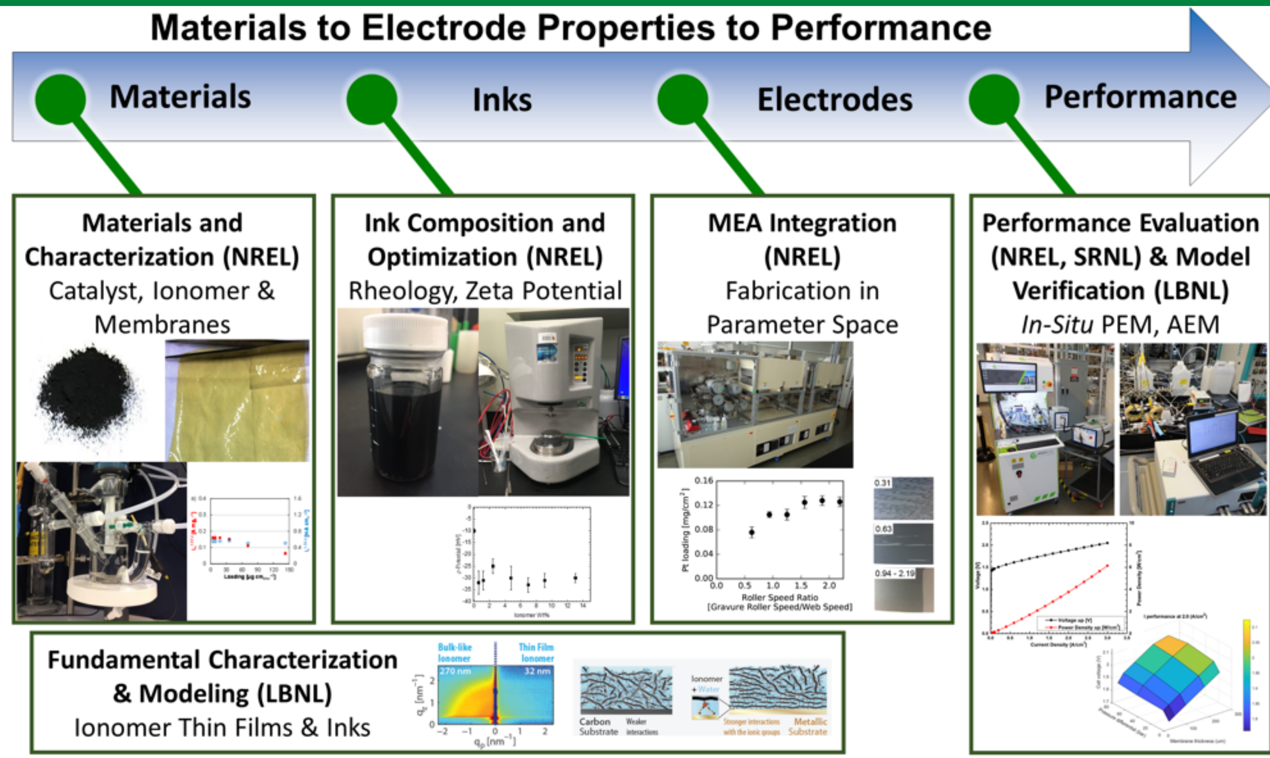


Supernodes Objectives:

- Combine/integrate nodes to demonstrate value when connected (sum greater than combination of individual parts)
- Increase collaboration across core labs
- Provide core research for EMN labs, beyond just project support

1. LTE/Hybrid Supernode: Linking Low-Temperature Electrolysis (LTE)/Hybrid Materials to Electrode Properties to Performance (NREL, SRNL, LBNL; 8 Nodes)

Goals: Create true understanding between ex-situ and in-situ performance. Identify how material properties are linked to electrode properties and how these are linked to electrolyzer performance.

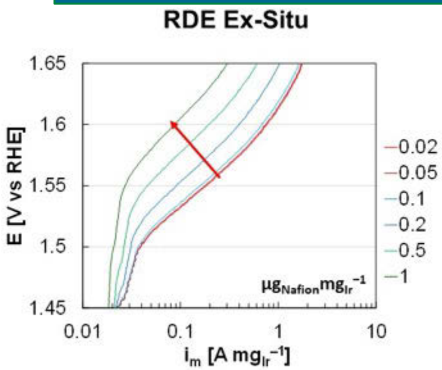


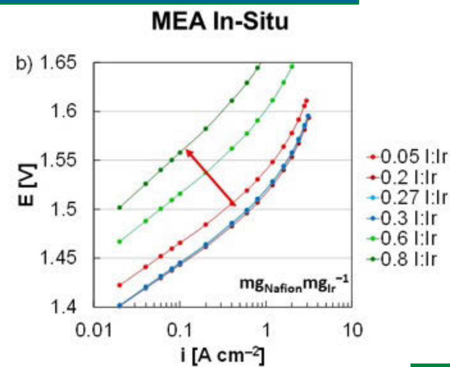
Outcome*: Better integration between ex-situ and in-situ performance, more relevant ex-situ testing, and improved material specific component development to achieve optimized electrolyzer cell performance and durability.*

1. LTE/Hybrid Supernode Accomplishments: RDE/MEA Correlation, Multiscale Modeling, and Scalable Coating Methods

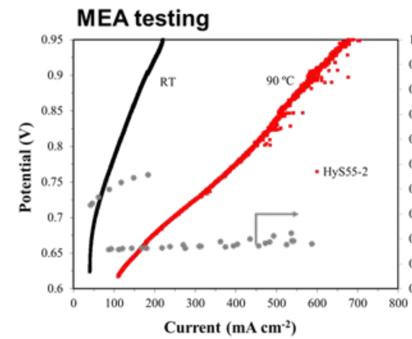
Correlation between RDE and MEA systems confirmed for LTE and Hybrid Cycle

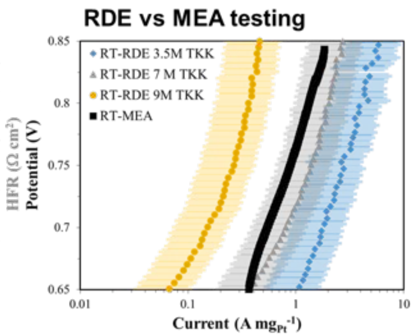
LTE



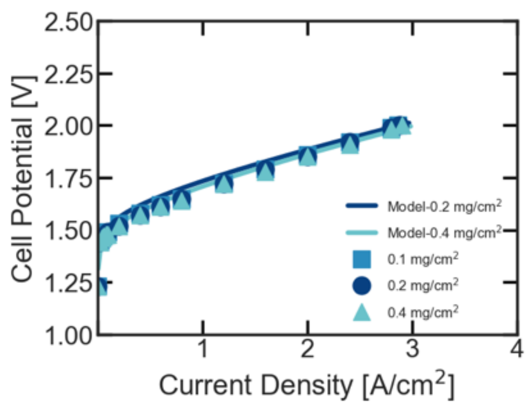


Hybrid Cycle

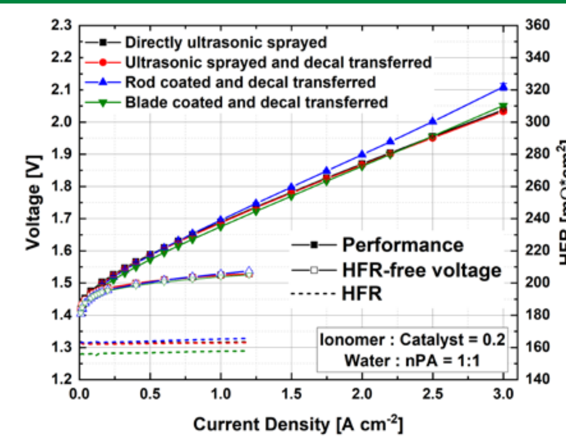




Multiscale modeling agrees with experimental data



Scalable coating methods (doctor blade) show comparable performance to lab-scale coatings (ultrasonic spray)

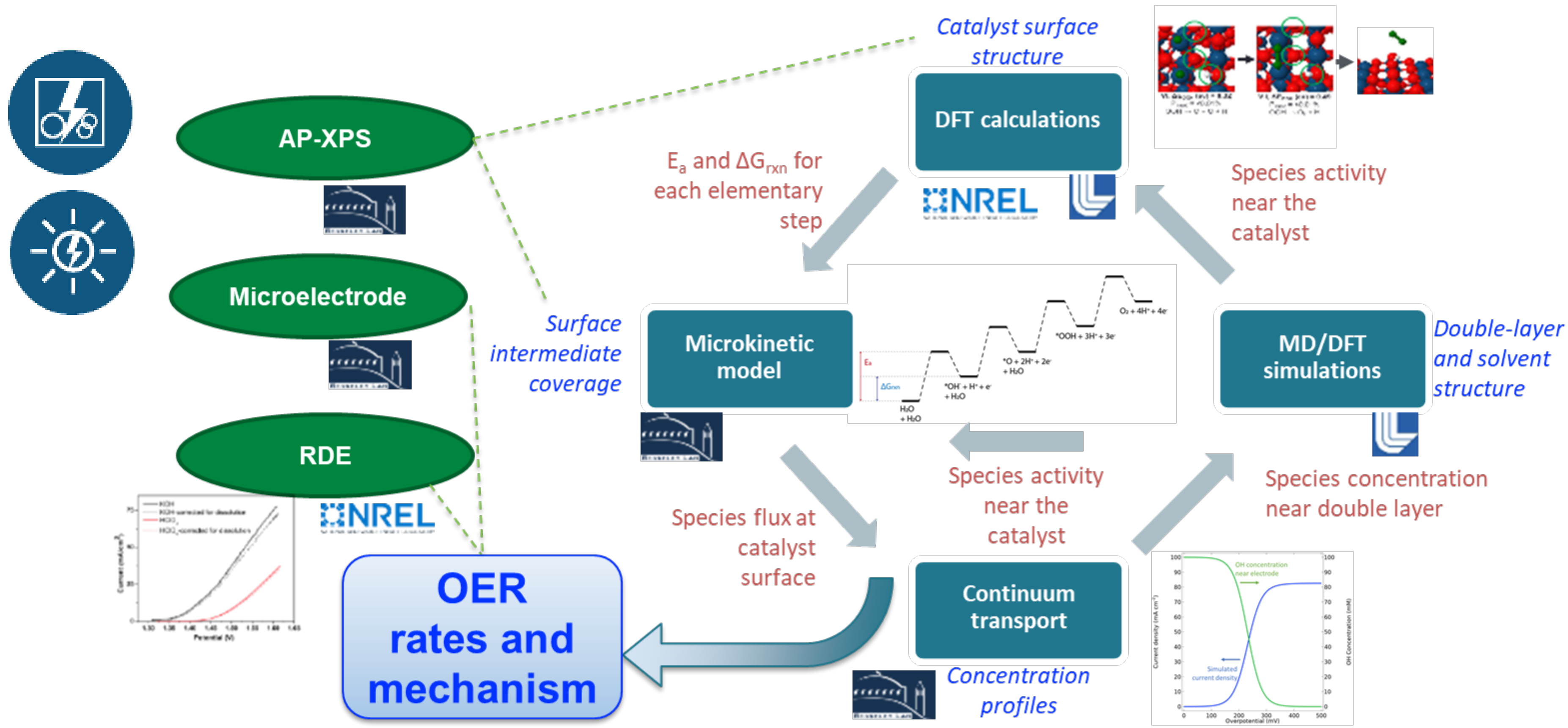


S.M. Alia, G.C. Anderson, *J. Electrochem. Soc.*, **2019**, *166*(4), F282-F294. DOI:10.1149/2.0731904jes

S. M. Alia, S. Stariha and R. L. Borup, J. Electrochem. Soc., **2019**, 166(15), F1164. DOI: 10.1149/2.0231915jes

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

***Goal:** Utilize validated theory across length scales to understand the mechanism of oxygen evolution going from acid to neutral to alkaline pH.*
Provide critical analysis for both LTE and PEC technologies



2. OER Supernode Accomplishment: Applied Multi-Scale Theories to Model OER Mechanism across pH Scales and Validated Experimentally on IrO_2

Atomistic Modeling (DFT, NREL)

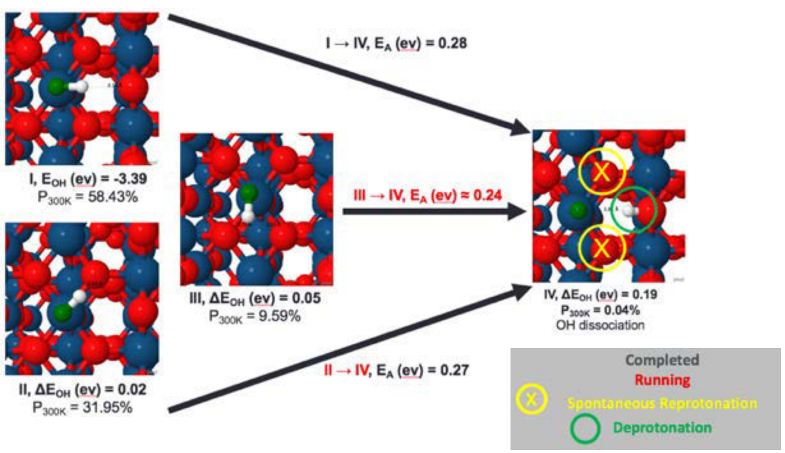
- Explore reaction mechanisms how to determine barriers

1. Bare Ir Surface

- Low O coverage limit (multiple pathways)
- High O coverage limit (thermodynamically favored)

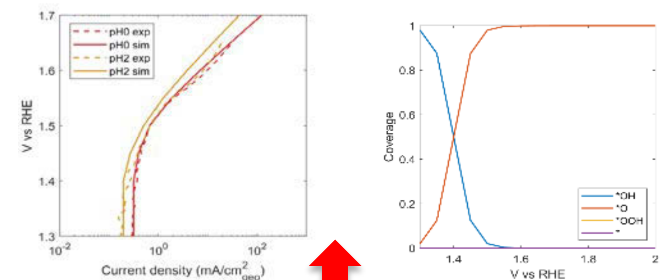
2. IrO_2 Surface from Pourbaix Analysis

- Established a way to determine intermediates, energetics and kinetics of OER
- Improved *ab-initio* Pourbaix diagram
- Refining transition states with *ab-initio* simulations
- Method to examine effects of solvation established



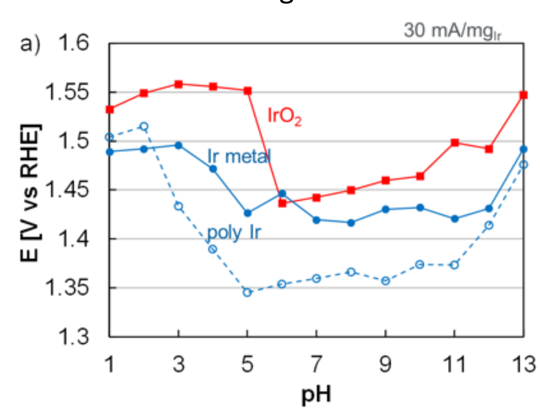
Microkinetic Modeling (LBNL)

- Use barriers from DFT and MD calculations to model OER rate and pathways, including mass transports
- Good agreement for low pH
- Surface coverages



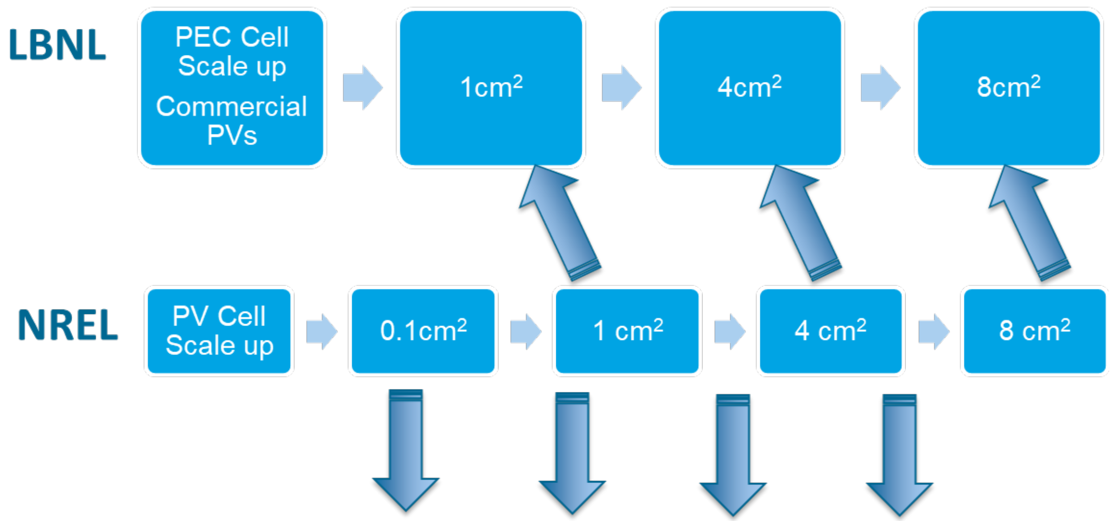
Experimental RDE Results (NREL)

- For Ir metal, activity improvement extended into weakly basic pH
- Activity dropped at pH 0/14, may be due to contaminants at higher concentrations



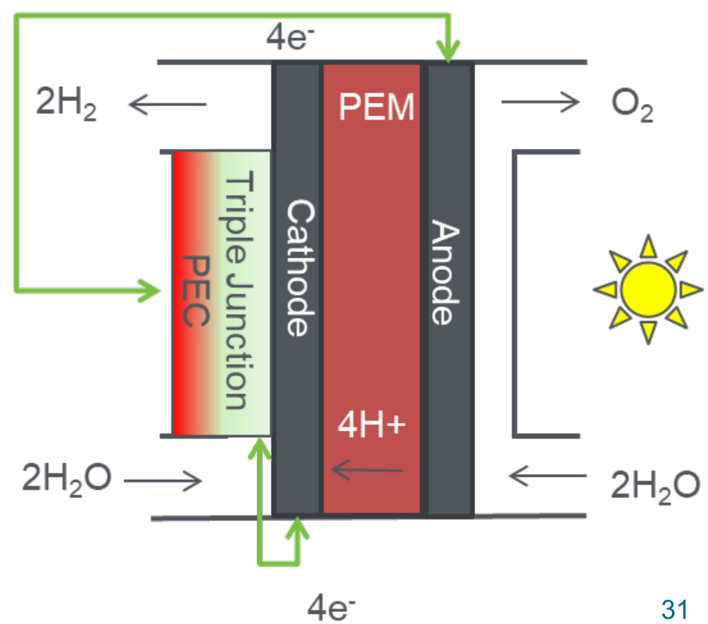
3. PEC Supernode: Emergent Degradation Mechanisms with Integration and Scale Up of PEC Devices (NREL, LBNL; 7 Nodes)

***Goal**: Understand integration issues and emergent degradation mechanisms of PEC devices at relevant scale and demonstrate an integrated and durable 50 cm^2 PEC panel.*



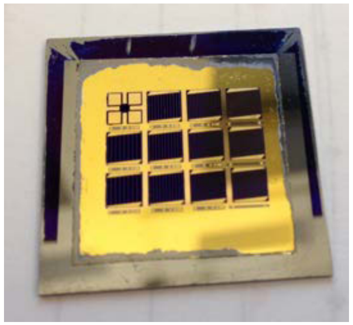
- **Benchmarking**
- ***In situ* degradation and characterization**
- **Emerging degradation pathways**
- **Modeling**

Integrated Photoelectrochemical

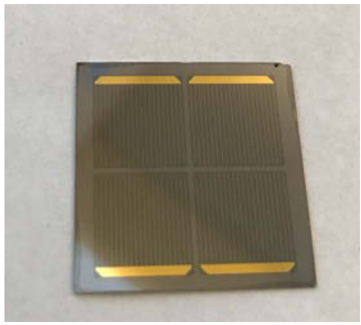


3. PEC Supernode Accomplishments: Fabrication, Cell Design, and On Sun PEC Testing Scale Up

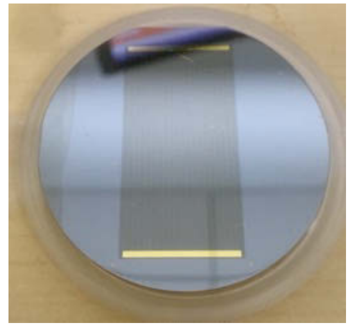
PEC Fabrication: GaInP/GaAs cells with 0.1 to 8-cm^2



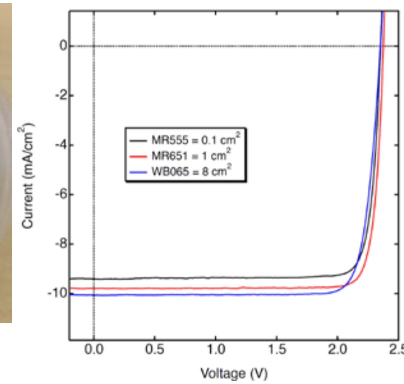
PV cells: ~0.1 cm^2



~1 cm^2

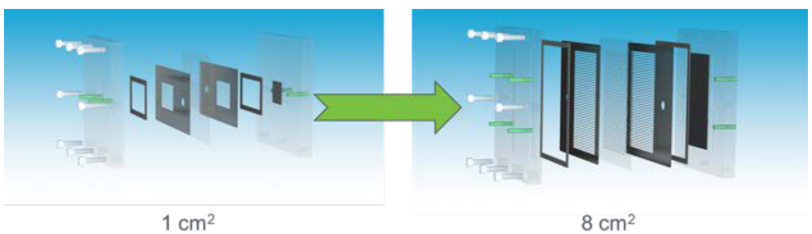


8 cm^2



- **These are the largest area III-V tandem cells made at NREL, enabling larger area PEC studies.**
- Significant effort toward developing growth recipes for uniform and high-quality GaInP.

Scale Up Towards 8-cm^2 Illuminated Area

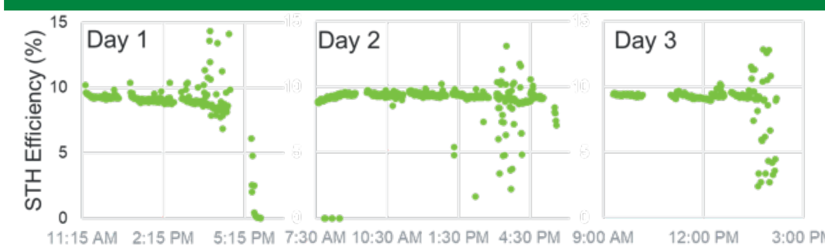


Degradation Modes Observed: 8-cm^2 Cell

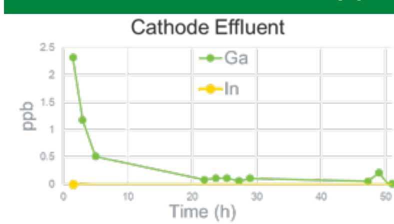
- **Gold grid finger delamination**
- **Anti-reflective coating dissolution**
- **Bubbles in epoxy – more light scattering**
- **Blistering**

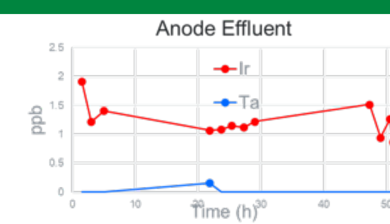
On Sun Durability Testing: 8-cm^2 Cell

- ***Test Duration:* 2 days, 2 hours, and 50 minutes**
- **Steady-state STH efficiency was 9.2%**



ICP-MS analysis of effluent showed Ga in cathode and 1-2 ppm Ir in anode





4. HTE Supernode: Characterization of Solid Oxide Electrode Microstructure Evolution (INL, NREL, LBNL, LLNL, Sandia; 7 Nodes)

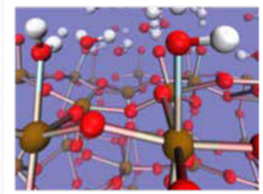
***Goal**: Deeper understanding of high-temperature electrolysis (HTE) electrode microstructure evolution as a function of local solid oxide composition and operating conditions.*

***Impact**: Comprehensive platform of HTE science and technology available for rapid utilization by HTE developers.*

Need: integrated, diverse set of capabilities and expertise, coordinated to develop a comprehensive understanding of HTE

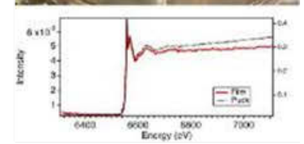
SNL: Imaging Node

LLNL: Modeling Node

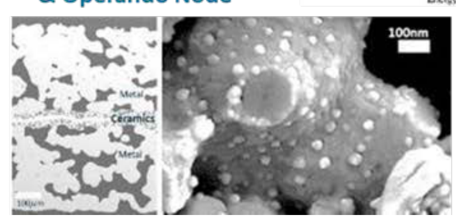


INL: Fabrication and Testing Node

NREL: Surface & Interface Node



LBNL: Processing & Operando Node

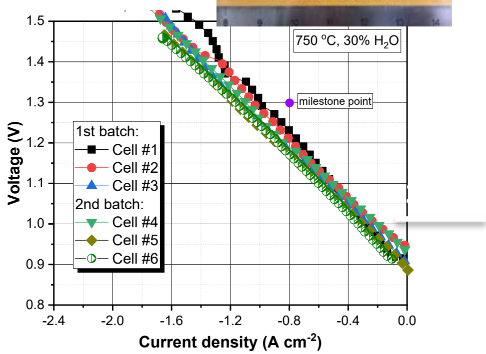


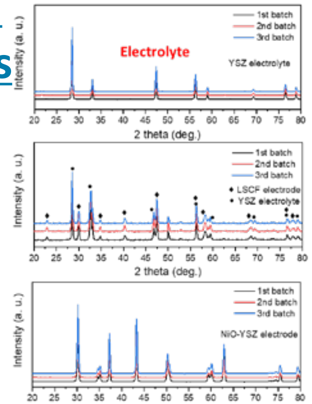
7 nodes combined: INL, NREL, LBNL, LLNL, SNL

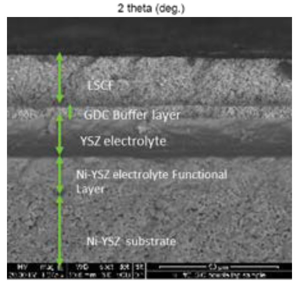
4. HTE Supernode Accomplishment: Cell Quality Control, Synchrotron Characterization, and Multiscale Microstructure Modeling Framework

Demonstrated quality control of R2R cell fabrication process (5 layers in cell) (INL)

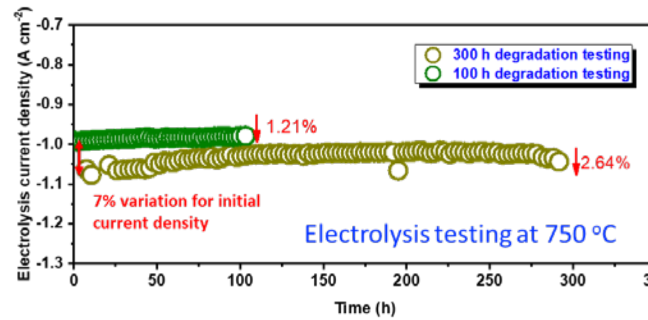
- Confirmed reproducibility of phase purity (XRD), structure (SEM) and SOEC performance of YSZ-based reference cells



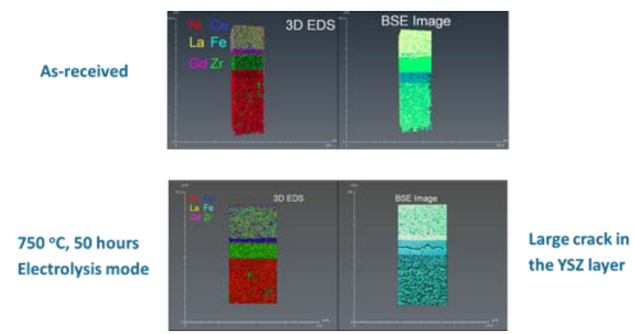




Understanding degradation mechanisms: Long-term SOEC testing (1.4 V) and post-mortem samples analysis (INL)

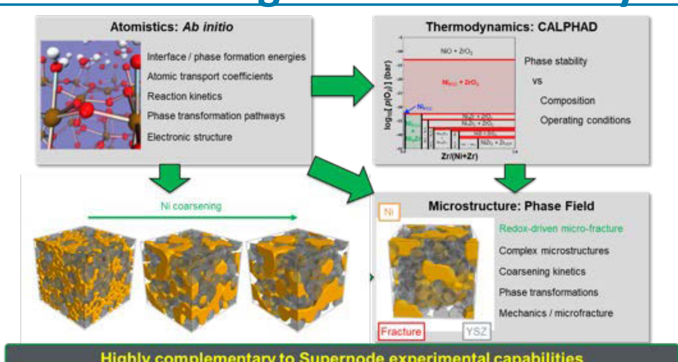


- **3D compositional analysis has been performed on as-received and cycled (SNL)**



- **Analyze representative HTE cell layers and interfaces with high precision at SLAC (NREL)**
  - Development of secondary phases (XRD)
  - Interdiffusion of elements (XRD, XAS, XRF)
  - Formation of voids (tomography - TXM)
- **ALS tomography, microdiffraction, non-ambient diffraction (LBNL)**

Develop a new computational tool to predict microstructure degradation in HTE systems (LLNL)



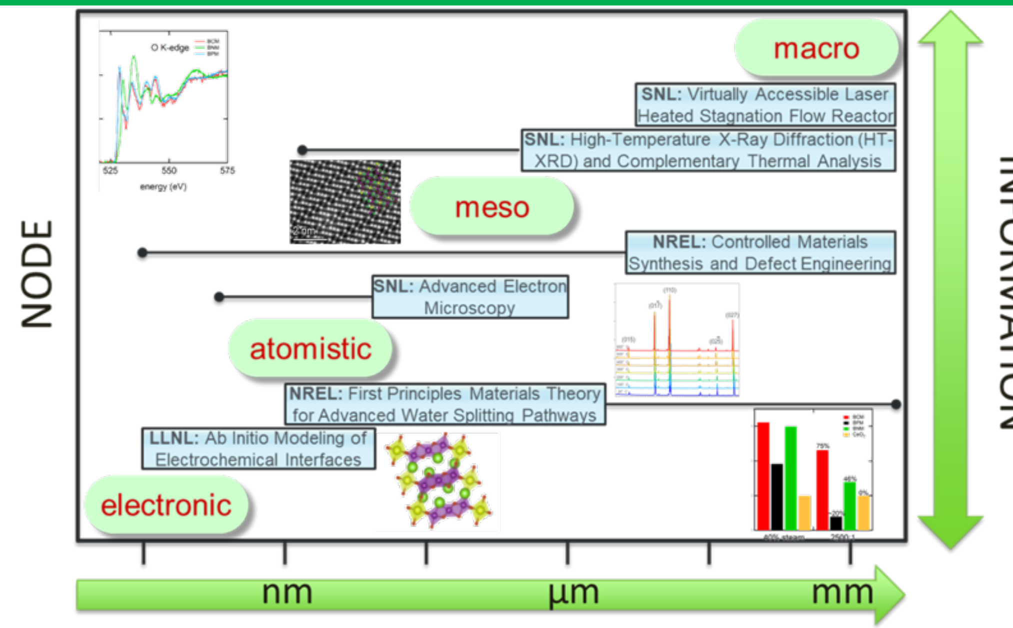
5. STCH Supernode: Develop Atomistic Understanding of Layered Perovskite $Ba_4CeMn_3O_{12}$ (BCM) and its Polytypes (LLNL, NREL, SNL; 6 Nodes)

***Goal**: Develop a fundamental understanding of how unique electronic structures, induced by Mn-O ligand bond arrangements, influence favorable water-splitting material behavior.*

***Impact:** Discover new STCH materials capable of splitting water at high H_2O:H_2 ratio. Knowledge gained here supports FOA-awarded projects' goals.*

Important Interrelationships:

- electronics
- defects
- structure
- performance

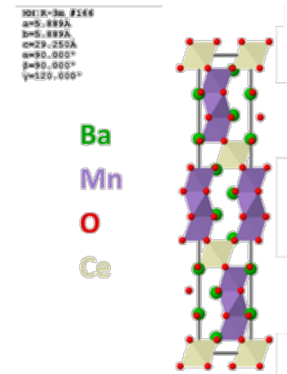


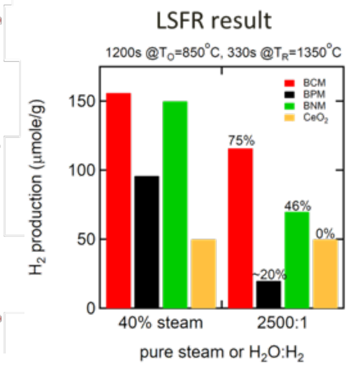
Objectives:

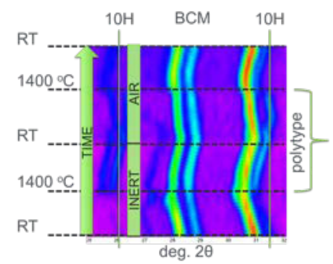
- Discover and synthesize model perovskite system
- Develop and exercise multi-length-scale observation platforms and methods
- Apply first principles theory to derive atomistic understanding of water splitting activity

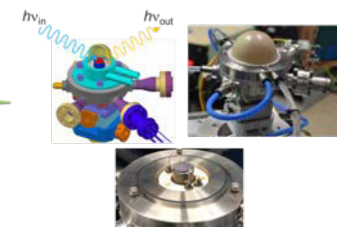
5. STCH Supernode Accomplishments: Discovered New Materials, Demonstrated Hydrogen Production, Developed Advanced Characterization

- Discovered **TWO** new water splitting compounds that are structurally identical and compositional variants to $Ba_4CeMn_3O_{12}$ (BCM).
  - Identical crystallography
  - Different electronic structure *and* water splitting behavior
- Demonstrated H_2 production capacity of new compounds exceeds CeO_2 cycled at T_R = 1350 °C.
- Developed research tools and validated methodology.
  - *In situ* hot stage EELS and high-resolution electron microscopy
  - Operando synchrotron X-ray scattering (SLAC)
  - Ab initio theory (defect thermodynamics)
- Generating foundational knowledge to correlate water splitting activity with electronic structure.

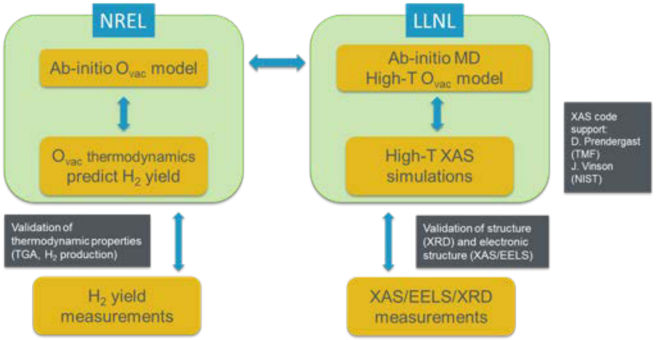








Atomistic Modeling of Scattering Experiments and Defect Chemistry



Accomplishments: HydroGEN Benchmarking Advanced Water Splitting Technologies Project (P170)

Best Practices in Materials Characterization

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

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

Accomplishments:

- 2nd 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

Responses to Previous Year Reviewers' Comments

- As the consortium matures, it may be helpful to establish formal internal mechanisms for self-assessment, deciding future directions, identifying existing barriers, and selecting concrete steps to take to overcome these to maximize the impact of the nodes and ensure adaptability.

Response: We agree. While these activities are not overtly described or the results summarized in the AMR presentation, the HydroGEN Steering Committee along with guidance from DOE does have internal mechanisms in place to self-assess and take action to maximize consortium effectiveness. While the labs do provide input about future directions, defining and implementing is DOE's purview. An example of how we have done this is developing the Supernode concept. When we developed the Supernode concept, we identified the major barrier(s) for each of the AWS technologies. These barriers are not being addressed by the FOA-awarded projects and can only be tackled by the HydroGEN labs because of labs' existing expertise and capabilities. Each Supernode involves multi-lab and multi-node collaboration, has high impact goals and outcomes, and has concrete steps to overcome these barriers.

- By managing the materials characterization within the national laboratory complex, HydroGEN helps industrial–academic teams focus on making progress toward their performance and durability targets.

Response: We agree. The EMN approach leverages the world-class materials characterization capabilities within the national laboratory complex and enables scientific progress in a way that would probably not be achieved by a small project working independently. This materials characterization capability and AWS expertise within the national labs also point to the fact that a good role for the national labs would be to validate and benchmark materials.

Responses to Previous Year Reviewers' Comments

- Within the results presented, the strong collaboration between the project partners and other R&D peers across the community is clear to see. However, it is recommended that a list of achieved publications be presented so that the multi-laboratory collaboration within HydroGEN and with other institutions can be easily identified.

Response: A list of achieved publications (24) and presentations (88) were included in the "Reviewers-Only Slides" section. A list of patents and patent applications were also included in the same section. Furthermore, we are developing a new publications search engine on the www.h2awsm.org website to list publications that pulls directly from H2AWSM Zotero library.

- It is difficult to put in perspective to what extent the accomplishments presented have moved each of the four technologies toward meeting the $2/kg goal. Furthermore, it is difficult to put in perspective where each of the four technologies stands relative to meeting the $2/kg goal. While it is not necessarily a weakness, it would be beneficial to understand how the funding is allocated among the four water-splitting technologies, with which of the four technologies the nodes being utilized align, from which technology data is being accessed, etc. This understand would provide a better understanding of how the capabilities, expertise, and R&D for each technology is being utilized.

Response: The funding is equally allocated among the four water splitting technologies. This is indicated by the same number of projects awarded for each technology as each project received a similar amount of funding. The technology-specific posters and the individual project presentations illustrate how the HydroGEN capability nodes, expertise, and R&D are being utilized.

Proposed Future Work

- Core labs will execute HydroGEN lab nodes to enable successful phase 2 and 3 project activities and work with new phase 1 projects
  - Core labs' interaction with a specific project will end if that project does not achieve its go/no-go decision metric
- Foster growth of phase 2 Supernode work and continue to collaborate and perform integrated research in the five Supernodes to accelerate AWS research
- Work closely with the Benchmarking Team to establish benchmarking, standard protocols, and metrics for the different water-splitting technologies
- Continue to develop a user-friendly, secure, and dynamic HydroGEN Data Hub that accelerates learning and information exchange within the HydroGEN EMN labs, their partners, and other EMN, AE, PEC, and STCH communities
  - Implement advanced data tool infrastructure improvements and capabilities for more open collaboration and contributions across the HydroGEN consortium, including developing additional data harvesting tools that integrate lab data systems with Data Hub services
- Continue to develop a user-friendly, information rich, and relevant HydroGEN website and implement the publication page
- Outreach

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

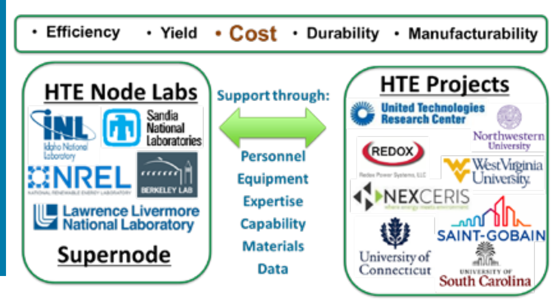
Summary—HydroGEN Consortium: Advanced Water-Splitting Materials (AWSM)

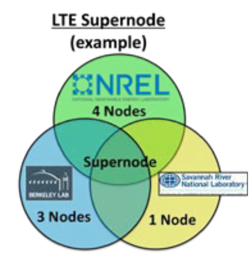
A Nationwide, Interagency, Collaborative Consortium in Early-Stage Materials R&D

>80 unique, world-class capabilities/expertise:

- *Materials theory/computation*
- *Synthesis*
- *Characterization and analysis*

- 19 projects successfully passed GNG
- 5 Supernodes passed GNG
- 4 NSF DMREF projects completed
- 11 new Round 2 FOA projects started
- 1 MRS TV HydroGEN video
- 2 annual benchmarking workshops
- 36 AWS standard protocols
- Data Hub >36,500 files, 258 users
- Implemented data governance processes





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

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HydroGEN
Advanced Water Splitting Materials

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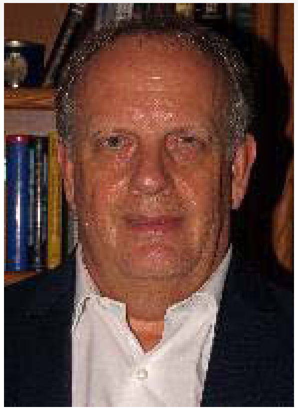
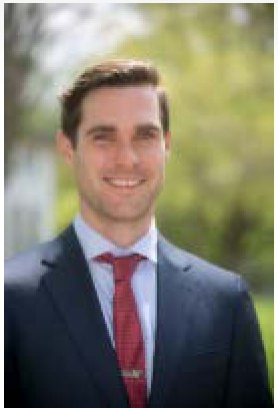


Ned Stetson

Katie Randolph

David Peterson



James Vickers

Eric Miller

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

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Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

NREL Team

Huyen Dinh, Lead

Principal Investigators:

Shaun Alia	Zhiwen Ma
Mowafak Al-Jassim	Scott Mauger
Guido Bender	Kristin Munch
Joe Berry	Judy Netter
Jeff Blackburn	Craig Perkins
Todd Deutsch	Bryan Pivovar
Myles Steiner	Matthew Reese
David Ginley	Genevieve Saur
Mai-Anh Ha	Glenn Teeter
Kevin Harrison	Michael Ulsh
Steven Harvey	Judith Vidal
Stephan Lany	Andriy Zakutayev
Ross Larsen	Kai Zhu

LBNL Team

Adam Weber, Lead

Principal Investigators:

Nemanja Danilovic	Francesca Toma
Peter Agbo	Miquel Salmeron
Jason Cooper	Ethan Crumlin
David Larson	Ahmet Kusoglu
Lin-Wang Wang	Frances Houle
Walter Drisdell	David Prendergast
Michael Tucker	Ravi Prasher
Jinghua Guo	Hanna Breunig

SRNL Team

Elise Fox, Lead

Principal Investigators:

Maximilian Gorensek   Brenda L. Garcia-Diaz

Hector Colón-Mercado

NREL — BERKELEY LAB — Sandia National Laboratories — INL Idaho National Laboratory — Lawrence Livermore National Laboratory — SRNL

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Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

SNL Team

Anthony McDaniel, Lead
Principal Investigators:

Andrea Ambrosini
Mark Allendorf
Eric Coker
Bert Debusschere
Farid El Gabaly
Lindsay Erickson
James Foulk
Cy Fujimoto
Fernando Garzon
Ethan Hecht
Cliff Ho
Reese Jones
Bryan Kaehr
David Littlewood
John Mitchell
Jeff Nelson
Peter Schultz
Randy Schunk
Subhash Shinde
Josh Sugar
Alec Talin
Alan Wright
Kevin Albrecht

LLNL Team

Tadashi Ogitsu, Lead
Principal Investigators:

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

INL Team

Richard Boardman, Lead
Principal Investigators:

James O'Brien
Dong Ding
Rebecca Fushimi
Dan Ginosar
Gary S. Groenewold
Hanping Ding
Gabriel Ilevbare

NREL — Berkeley Lab — Sandia National Laboratories — INL Idaho National Laboratory — Lawrence Livermore National Laboratory — SRNL

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Technical Backup Slides

LTE Projects

2017 FOA Projects:

1. **Proton Onsite** - High Efficiency **PEM** Water Electrolysis Enabled by Advanced Catalysts, Membranes and Processes
2. **Argonne National Laboratory** - PGM-free OER Catalysts for **PEM** Electrolyzer
3. **Los Alamos National Laboratory** - Scalable Elastomeric Membranes for **Alkaline** Water Electrolysis
4. **Los Alamos National Laboratory** - High-Performance Ultralow-Cost Non-Precious Metal Catalyst System for **AEM** Electrolyzer
5. **Northeastern University** - Developing Novel Platinum Group Metal-Free Catalysts for **Alkaline** Hydrogen and Oxygen Evolution Reactions

2019 FOA Projects:

1. **Georgia Institute of Technology** - Interface and Electrode Engineering for Durable, Low Cost **Alkaline** Anion Exchange Membrane Electrolyzers
2. **The Chemours Company FC, LLC** - Performance and Durability Investigation of Thin, Low Crossover **Proton Exchange Membranes** for Water Electrolyzers
3. **University of Oregon** - Pure Hydrogen Production through Precious-Metal Free **Membrane** Electrolysis of Dirty Water

HTE Projects

2017 FOA Projects:

1. **Saint-Gobain -** Development of Durable Materials for Cost Effective Advanced Water Splitting Utilizing All Ceramic **Solid Oxide Electrolyzer** Stack Technology
2. **United Technologies Research Center** - Thin Film, Metal-Supported, High Performance, and Durable **Proton-Solid Oxide Electrolyzer Cell**
3. **University of Connecticut** - **Proton-Conducting Solid Oxide Electrolysis** Cells for Large-Scale Hydrogen Production at Intermediate Temperatures
4. **West Virginia University** - Intermediate Temperature **Proton-Conducting Solid Oxide Electrolysis** Cells with Improved Performance and Durability
5. **Northwestern University -** Characterization and Accelerated Life Testing of a New **Solid Oxide Electrolysis Cell**

2019 FOA Projects:

1. **Nexceris, LLC** - Advanced Coatings to Enhance the Durability of **SOEC** Stacks
2. **Redox Power Systems, LLC** - Scalable High-H_2 Flux, Robust Thin Film **Solid Oxide Electrolyzer**
3. **University of South Carolina** - A Multifunctional Isostructural Bilayer Oxygen Evolution Electrode for Durable Intermediate Temperature Electrochemical Water Splitting

STCH Projects

2017 FOA Projects:

1. **Arizona State University** - Mixed Ionic Electronic Conducting Quaternary Perovskites: Materials by Design for STCH H_2
2. **Colorado School of Mines** - Accelerated Discovery of STCH Hydrogen Production Materials via High-Throughput Computational and Experimental Methods
3. **Northwestern University** - Transformative Materials for High-Efficiency Thermochemical Production of Solar Fuels
4. **University of Colorado Boulder** - Computationally Accelerated Discovery and Experimental Demonstration of High-Performance Materials for Advanced Solar Thermochemical Hydrogen Production
5. **Greenway Energy** - High Temperature Reactor Catalyst Material Development for Low Cost and Efficient Solar Driven Sulfur-Based Processes (Hybrid Sulfur)

2019 FOA Projects:

1. **University of California, San Diego** - New High-Entropy Perovskite Oxides with Increased Reducibility and Stability for Thermochemical Hydrogen Generation
2. **University of Florida** - A New Paradigm for Materials Discovery and Development for Lower Temperature and Isothermal Thermochemical H2 Production

PEC Projects

2017 FOA Projects:

1. **Stanford University** - Protective Catalyst Systems on III-V and Si-Based Semiconductors for Efficient, Durable Photoelectrochemical Water Splitting Devices
2. **Rutgers University** - Best-in-Class Platinum Group Metal-Free Catalyst Integrated Tandem Junction PEC Water Splitting Devices
3. **University of Michigan** - Monolithically Integrated Thin-Film/Si Tandem Photoelectrodes
4. **University of Hawaii** - Novel Chalcopyrites for Advanced Photoelectrochemical Water-Splitting

2019 FOA Projects:

1. **Rice University** - Highly Efficient Solar Water Splitting Using 3D/2D Hydrophobic Perovskites with Corrosion Resistant Barriers
2. **University of Toledo** - Perovskite/Perovskite Tandem Photoelectrodes for Low-Cost Unassisted Photoelectrochemical Water Splitting
3. **University of California, Irvine** - Development of Composite Photocatalyst Materials that are Highly Selective for Solar Hydrogen Production and their Evaluation in Z-Scheme Reactor Designs