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, D. Anton, R. Boardman, A. McDaniel, T. Ogitsu, A. Weber

Presenter: Huyen Dinh, NREL

Date: 4/30/2019

Venue: 2019 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: **$3.6M**
- FY18 DOE funding: **$9.9M**
- FY19 planned DOE funding: **$6.5M**
- Total DOE funding received to date: **$22M**

Barriers

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

Partners

NREL National Renewable Energy Laboratory

Berkeley Lab

Sandia National Laboratories

Lawrence Livermore National Laboratory

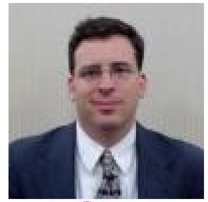
INL Idaho National Laboratory

SRNL

Collaboration: HydroGEN Steering Committee

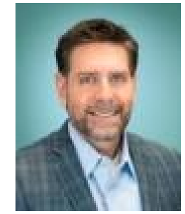
NREL
NATIONAL RENEWABLE ENERGY LABORATORY

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

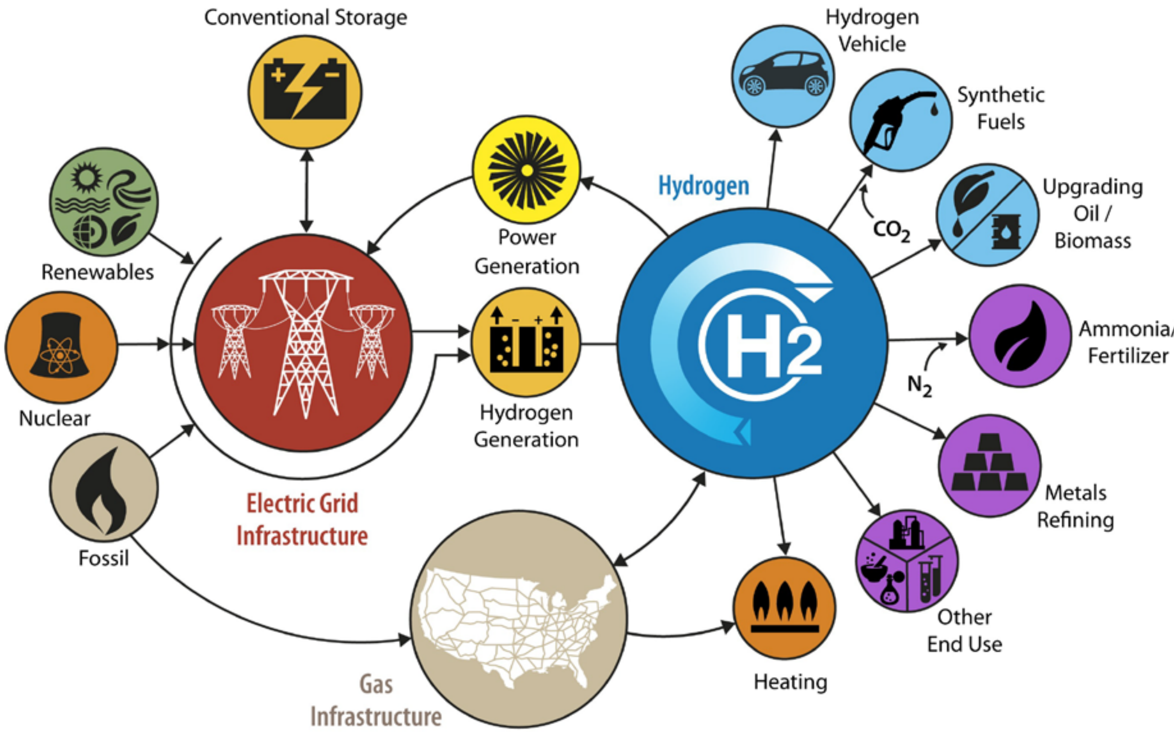
SRNL
SAVANNAH RIVER NATIONAL LABORATORY

Donald Anton

Eric Miller and Katie Randolph, DOE-EERE-FCTO

H2@Scale Energy System Vision
Relevance and Impact

Transportation & Beyond



*Illustrative example, not comprehensive

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

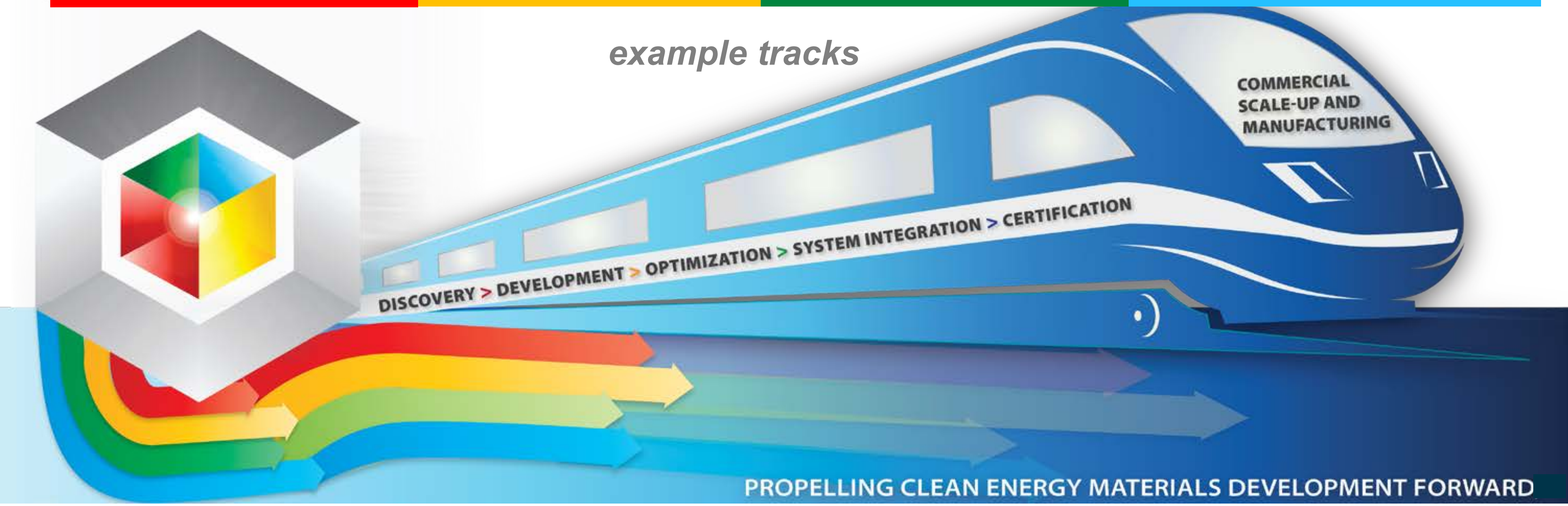
Materials innovations are key to enhancing performance, durability, and cost of hydrogen generation, storage, distribution, and utilization technologies key to H2@Scale

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

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
- INL (Idaho National Laboratory)
- 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:

Water →

- Photoelectrochemical (PEC)
- Solar Thermochemical (STCH)
- Low- and High-Temperature Advanced Electrolysis (LTE & HTE)

→ H H Hydrogen

H_2 Production target <$2/kg

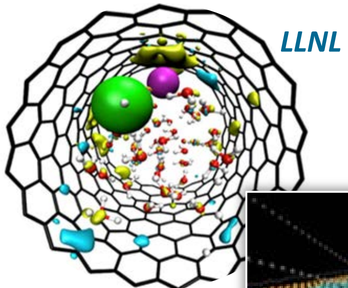
HydroGEN consortium supports early stage R&D in H_2 production

HydroGEN-AWSM Consortium

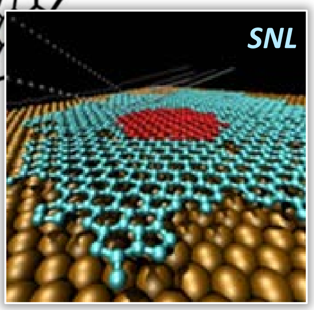
Relevance, Overall Objective, Impact, and Approach

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

Materials Theory/Computation

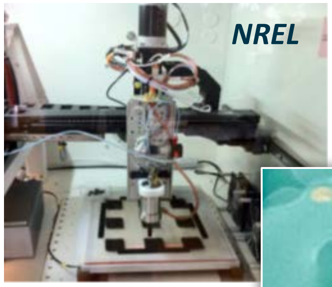


Bulk & interfacial models of aqueous electrolytes

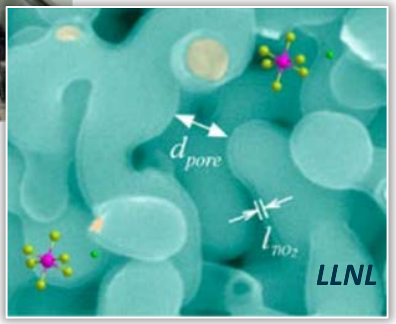


LAMMPS classic molecular dynamics modeling relevant to H_2O splitting

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

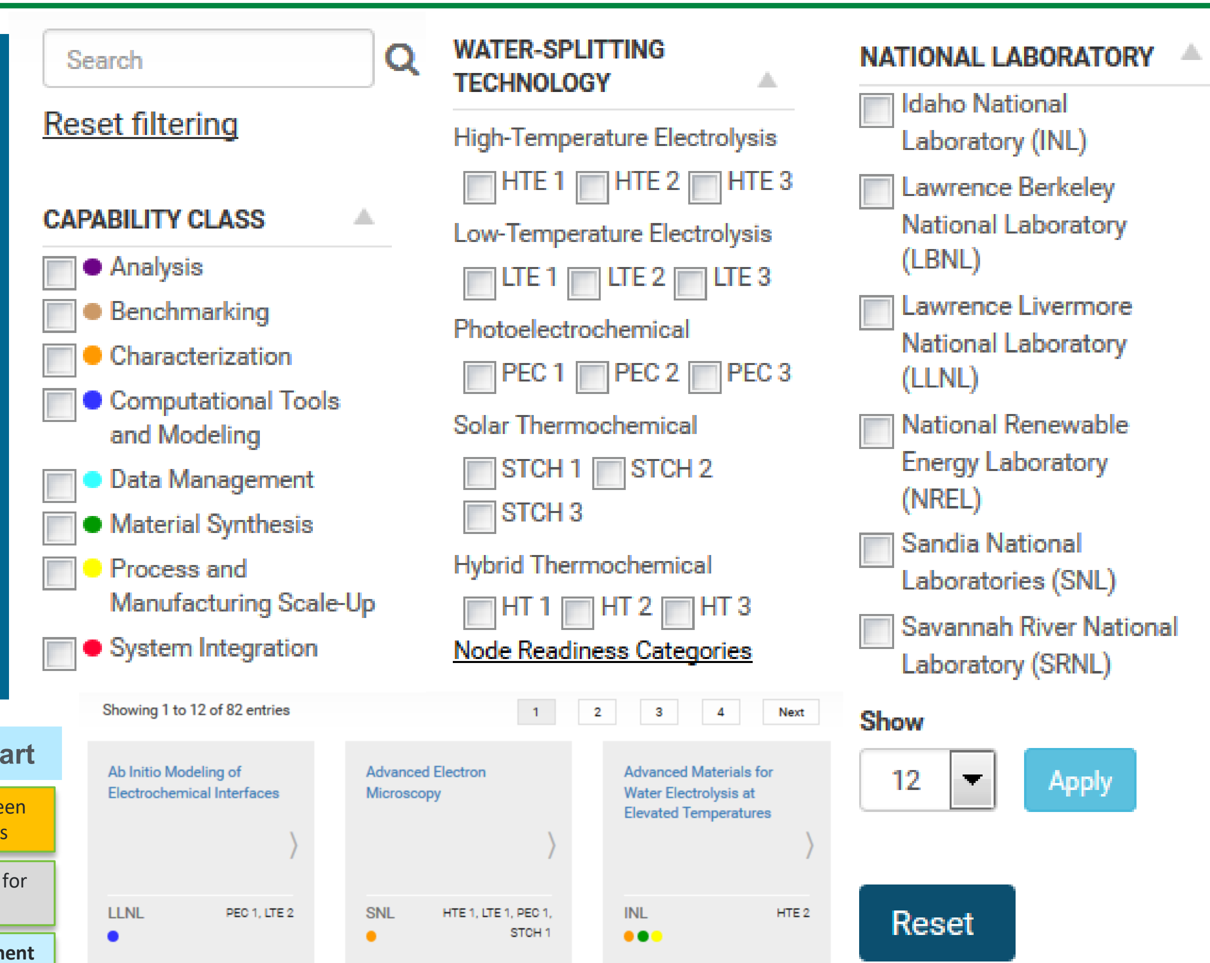
Website: https://www.h2awsm.org/

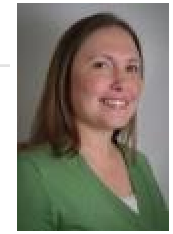
Accomplishments: Updated Capability Nodes on the User-Friendly Node Search Engine for Stakeholders

Added <u>3 new</u> and updated <u>>40 current</u> capability nodes:

- Hybrid Organic Inorganic Perovskites for Water Splitting
- Understanding catalyst inks and ionomer dispersions
- Electronic-Structure Modeling for Atomistic Understanding of Catalytic Materials with Real-World Distributions of Facets and Defects

Considered capability assessment from benchmarking team





Node Readiness Category (NRC) Chart

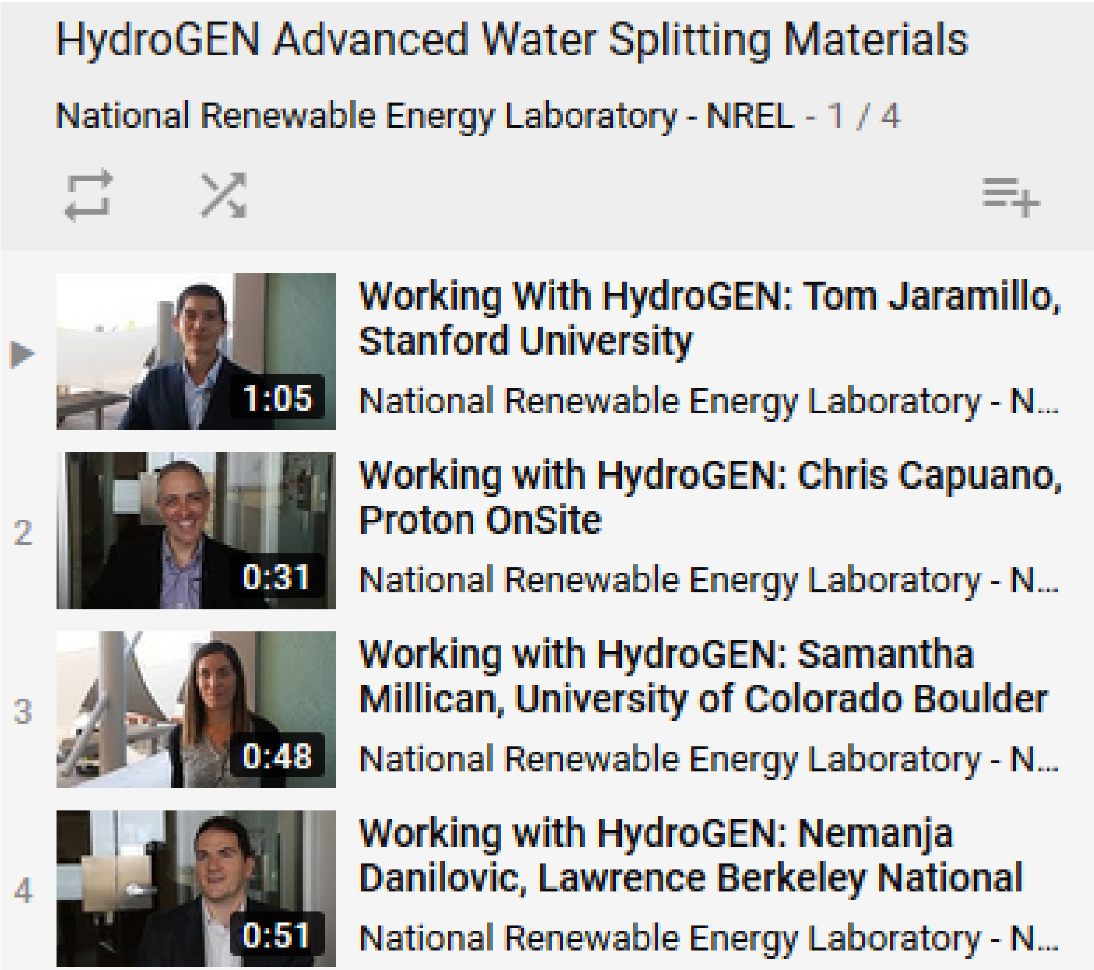
Node is **fully developed** and has been used for AWSM research projects

Node requires **some development** for AWSM

Node requires **significant development** for AWSM

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

Accomplishments: Maintained HydroGEN Website and Developed “Working with HydroGEN” Video Testimonials



Partner testimonial videos can be found here:
https://www.youtube.com/watch?v=1eK8ZnVo2Y&list=PL3GM1pjrYAchur4Aq1pojTC2cMPf8xs6P

WORKING WITH HYDROGEN: WHAT OUR PARTNERS SAY

Tom Jaramillo, principal investigator on a HydroGEN seedling project, talks about how the capabilities and expertise of the HydroGEN Advanced Water Splitting Materials consortium can help researchers working on hydrogen technologies.

4,373 users
24,011 pageviews
564 downloads

Visitors:
85% new
15% returning

Traffic:
46% search
37% direct
17% referral

Posted 10 news items

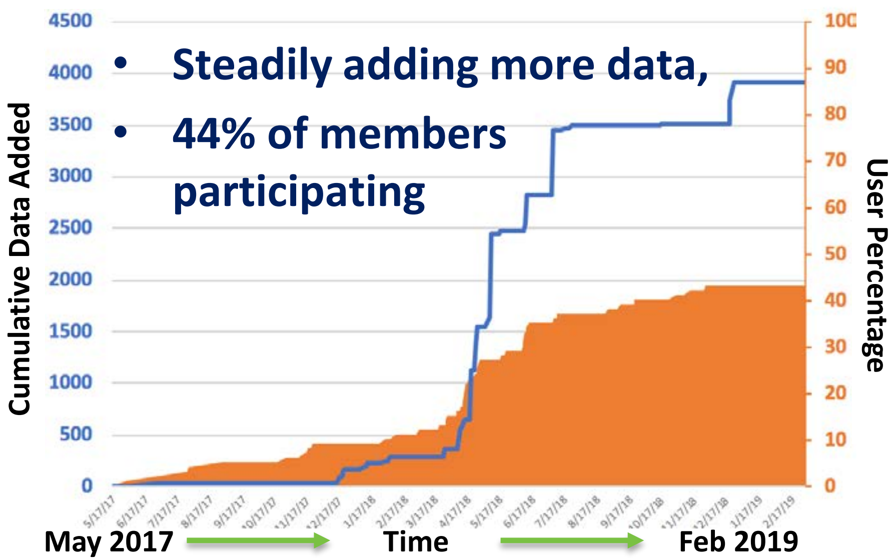
Added “Work with Us” page to top menu

Accomplishments:
HydroGEN Data Hub: Making Digital Data Accessible

https://datahub.h2awsm.org/

179 Users | **4055** Files

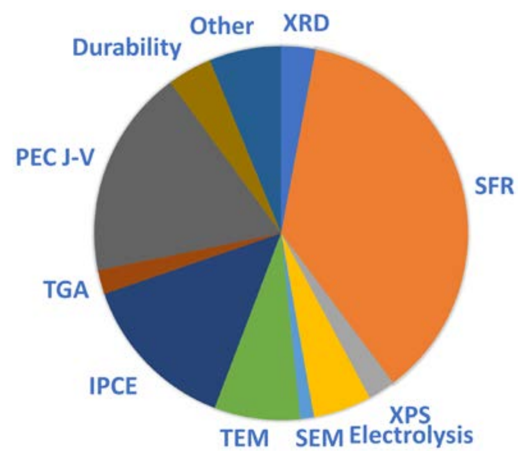
Cumulative Data on H2AWSM Data Hub



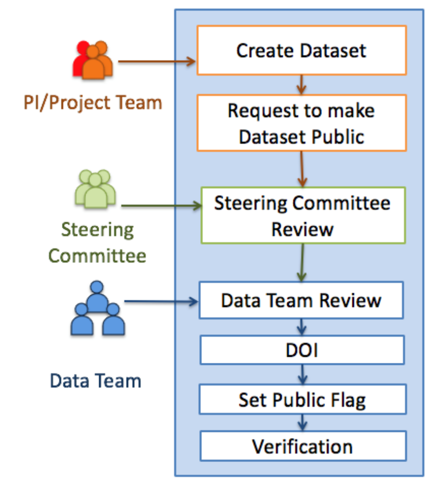
Data Hub implemented in May 2017

- Secure project space for team members
  - Centralized authentication
- Data publication process developed (FY2018Q3 QPM-see Reviewer-Only slides)
- Metadata tools and improvements to support advanced search

Types of Experimental Data



Data Publication Process



Data Team

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

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 Tools for Data Ingestion, Visualization and Analysis (Leveraging other EMNs)

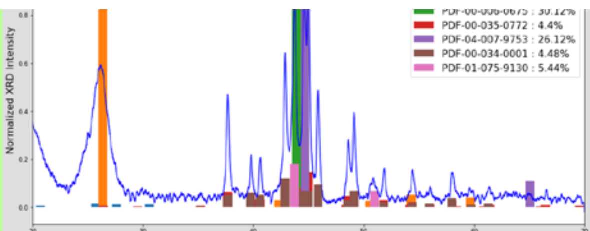
5 currently available, 5 under development

Simple data interface developed

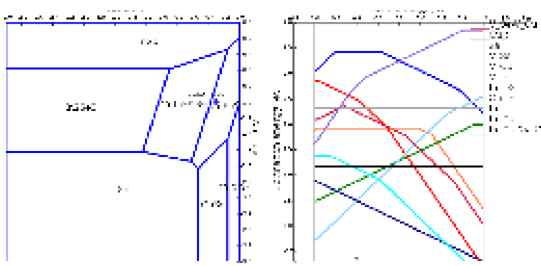
Materials properties

(A&V examples)

Structural information: XRD interface in collaboration with ElectroCat



Phase stability & Defect properties



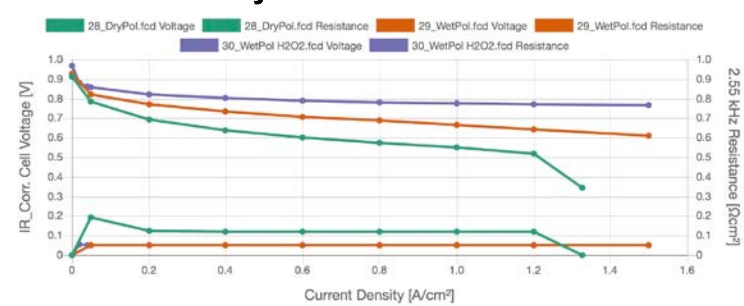
Data Tools for

- EMN collaboration
  - Data exchange and exploration
  - Data analysis and visualization (A&V)
- External users
  - Access to comprehensive database
    - Experimental and computational
  - Materials properties
    - Spectroscopy, phase stability, etc.
  - Device performance

Device performance

(A&V example)

Electrolysis Performance curve



Organically linked data and their representations

Accomplishments: Technology Transfer Agreements (TT/A)

➢ Streamlined Access

- ✓ **Four** standard, pre-approved TT/A between all consortium partners
- ✓ Executed all 21 project NDAs and 2 MTAs
- ✓ Updated multiple, more flexible CRADAs
  - Single Lab Single Participant
  - Multi-Lab Single Participant
  - Multi-Lab Multi-Participant
- ✓ Established Work For Others Agreements outside of FOA-awarded projects:
  - DeNora : GDE development on porous transport layers (LBNL Cell Testing Node)
  - German Aerospace Center: Concentrated solar power and solar fuels research (SNL)

Non-Disclosure Agreement (NDA) → Information Disclosure

Intellectual Property Management Plan (IPMP) → IP Protection

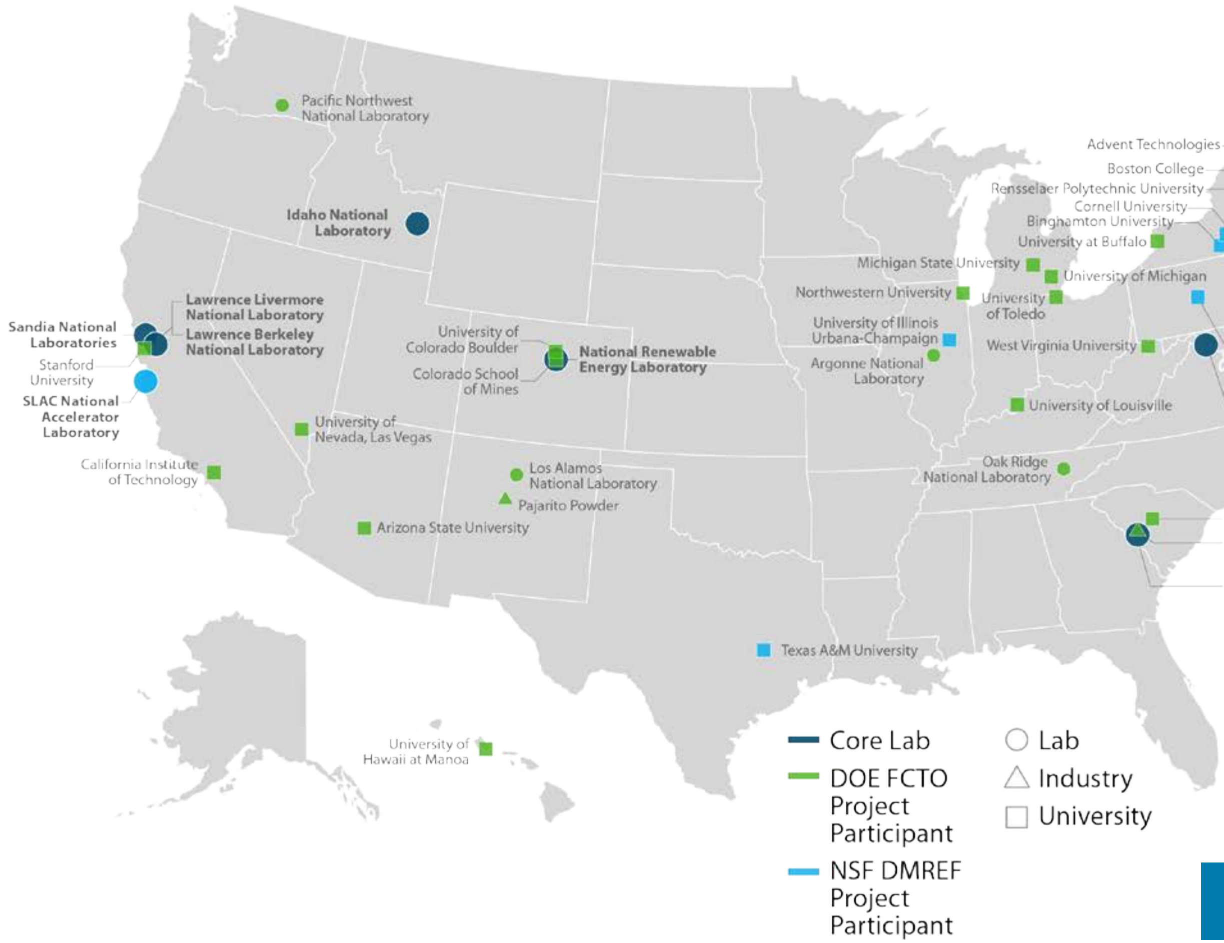
Materials Transfer Agreement (MTA) → Freedom to Operate

Cooperative Research and Development Agreement (CRADA) → Collaboration

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

National Innovation Ecosystem
Collaboration/Accomplishments

11 Labs **7** Companies **30** Universities **2** Funding Agencies



A Community Benchmarking Workshop

2 MRS Symposia

17 papers published

88 presentations

1 patent, 2 provisional applications filed; 1 SLAC proposal accepted

2 new HTE projects

5 new Supernodes

4 new NSF DMREF projects

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

4 New NSF DMREF/DOE EERE HydroGEN EMN Projects
Collaboration/Accomplishments

NSF DMREF PSU LTE (IA023 Poster)

PennState

Membrane Databases – New Schema and Dissemination

Recipient Penn State University (PI: Michael A. Hickner)

Subs National Institute of Standards and Technology/NIST (PI: Debra Audus) and Rensselaer Polytechnic Institute/RPI (PI: Chulsung Bae)

HydroGEN Node Experts

National Renewable Energy Laboratory:

- Shaun Alia
- Guido Bender
- Kristin Munch
- Bryan Pivovar

NSF DMREF CSM STCH (IA022 Poster)

School of Mines 1874 Colorado

High Temperature Defects: Linking Solar Thermochemcial and Thermoelectric Materials

Recipient Colorado School of Mines (PI: Eric Toberer and Vladan Stevanovic)

Subs University of Illinois Urbana-Champaign (PI: Elif Ertikin) and SLAC National Accelerator Laboratory (PI: Michael Toney)

HydroGEN Node Experts

National Renewable Energy Laboratory:

- Robert Bell
- David Ginley
- Stephan Lany
- Philip Parilla

NSF DMREF PSU PEC (IA024 Poster)

PennState

Experimental Validation of Designed Photocatalysts For Solar Water Splitting

Recipient Penn State University (PI: Ismaila Dabo and Raymond E. Schaak)

Subs Cornell University (PI: Héctor D. Abruña)

HydroGEN Node Experts

National Renewable Energy Laboratory:

- Todd Deutsch
- James Young

NSF DMREF UB PEC (IA021 Poster)

University at Buffalo
The State University of New York

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

Recipient University at Buffalo (PI: David Watson)

Subs Texas A&M University (PI: Sarbajit Banerjee) and Binghamton University (PI: Louis Piper)

HydroGEN Node Experts

Lawrence Berkeley National Laboratory

- Jinghua Guo
- David Prendergast

NSF = National Science Foundation;
DMREF = Designing Materials to Revolutionize and Engineer our Future

Collaboration: HydroGEN FOA-Awarded Projects

16 projects passed GNGs and in phase 2 + 2 new HTE projects awarded

49 unique capabilities being utilized across six core labs

Advanced Electrolysis (10)	PEC (5)	STCH (5)
LTE (5) HTE (5)	Benchmarking & Protocols (1)	2-Step MO_x(4) Hybrid Cycle (1)

A Balanced AWSM R&D Portfolio

Accomplishments/Collaborations

Low Temperature Electrolysis (LTE) (G. Bender: P148A; 5 Projects)

PEME Component Integration

PEM Electrolysis

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

AEM Electrolysis

High Temperature Electrolysis (HTE) (R. Boardman: P148B; 5 Projects)

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

O^{2-} conducting SOEC

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

H^{+} conducting SOEC

Photoelectrochemical (PEC) (A. Weber: P148C; 5 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) (A. McDaniel: P148D; 5 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

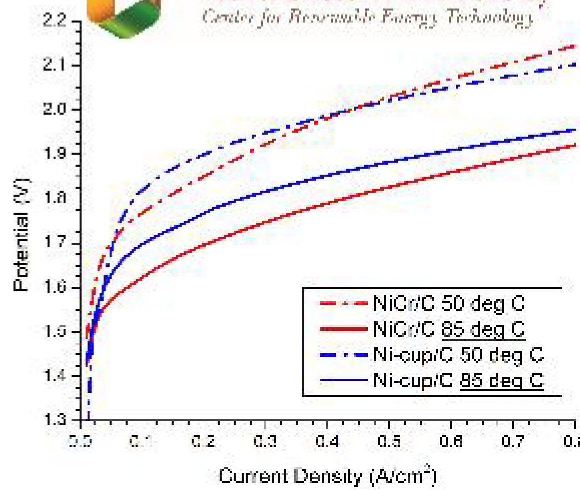
PGM = platinum group metal
Solid oxide electrolysis cells: SOEC

Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

Low Temperature Electrolysis (LTE)

NEU and UD demonstrated **high AEM electrolyzer performance (0.46 A/cm² at 1.8 V, 85°C),** using **PGM-free** Ni-Fe/Raney Ni OER and NiCr/C HER catalysts, PAP-TP-MQN AEM, and 1% K_2CO_3 solution, enabling durable, high-performing materials for efficient and low cost H_2 production. LBNL and SNL modeling nodes helped NEU better understand the AEM/catalyst interface, NREL nodes helped NEU characterize the membrane physical properties and optimize the catalyst formulation.

Northeastern University
Center for Renewable Energy Technology

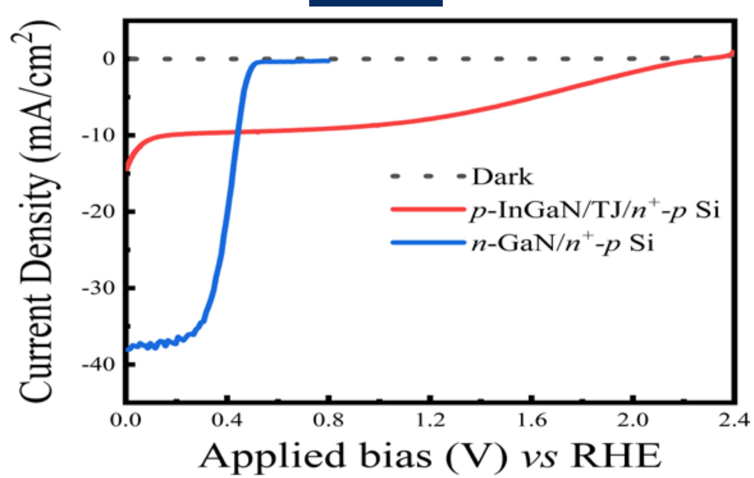


Anode: Ni-Fe/Raney Ni; Membrane: polyaryl piperidinyl triphenyl (PAP-TP-MQN), prepared by University of Delaware (UD)

Photoelectrochemical (PEC) Water Splitting

UM achieved a **first demonstration of a functional Si/InGaN tandem photoelectrode**. A **GaN/Si photocathode with stable operation (>100 h) at ~38 mA/cm², without using surface protection, was also demonstrated**. UM is focused on developing Si-based, low cost, high efficiency (>15%), and stable (>1,000 h) PEC tandem water splitting devices, using scalable, low cost semi-conductors, nanowire tunnel junction, and N-rich GaN self-protection. The photoelectrodes were characterized and optimized by the NREL and LBNL nodes, while LLNL carried out modeling to understand the protection role of N-rich GaN surfaces.

University of Michigan



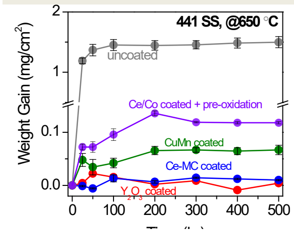
Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

High Temperature Electrolysis (HTE)

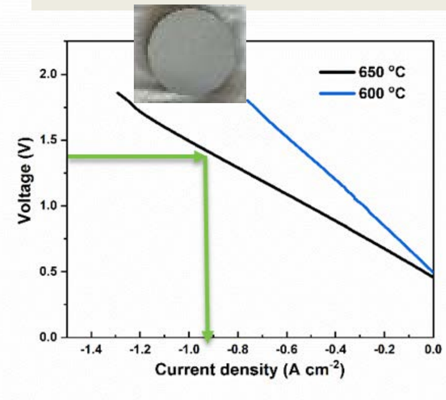
United Technologies Research Center (UTRC), with help from INL, LBNL , and NREL nodes, identified high performance proton-electrolytes and steam electrodes that resulted in **button cell performance exceeding the DOE performance target, stable protective coatings for 500 h**, and a cell model for SOEC performance characterization and cell/stack operation simulation. The HydroGEN nodes provided critical support by addressing technical barriers in metal alloy durability, electrode/electrolyte material optimization and stability, and SOEC modeling.

United Technologies Research Center

Protective coatings for SS alloys, 500h no oxidation

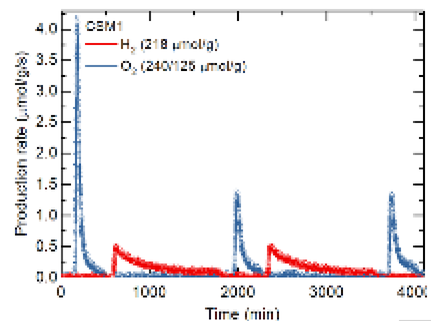


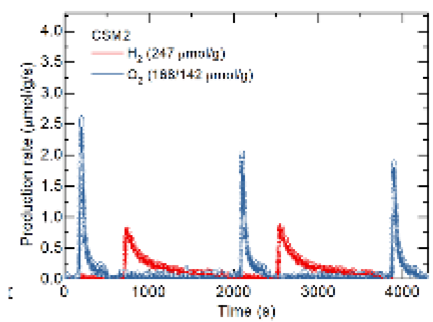
Button cell with SPS electrolyte exceeded BP1 target (>0.8 A/cm² at 1.4V & 650°C)



Solar Thermochemical (STCH) Water Splitting

CSM **exceeded its hydrogen production target of 59 μmol H_2/g sample by producing 218 and 247 μmol H_2/g using two compositions within $Ce_xSr_{2-x}MnO_4$ family**, x = 0.1 and 0.2, respectively. This promising performance further motivates the search for additional perovskite compounds with STCH water splitting properties. The objective is to discover new STCH materials that can meet steam to hydrogen efficiency of 20% and low cost H_2 production. The project leverages NREL and SNL modeling, material synthesis and characterization nodes.

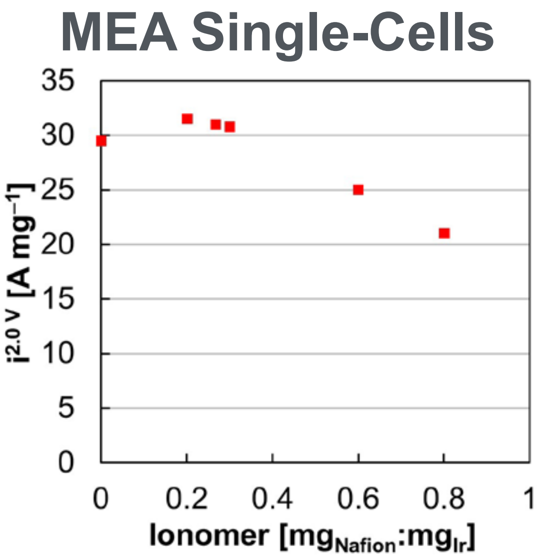


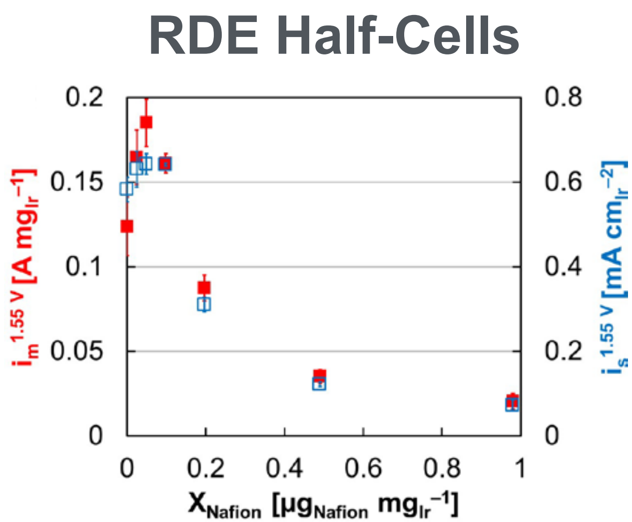


LTE/Hybrid Supernode: Linking LTE/Hybrid Materials to Electrode Properties to Performance (NREL, SRNL, LBNL; 8 Nodes)

***Goal**: 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.*

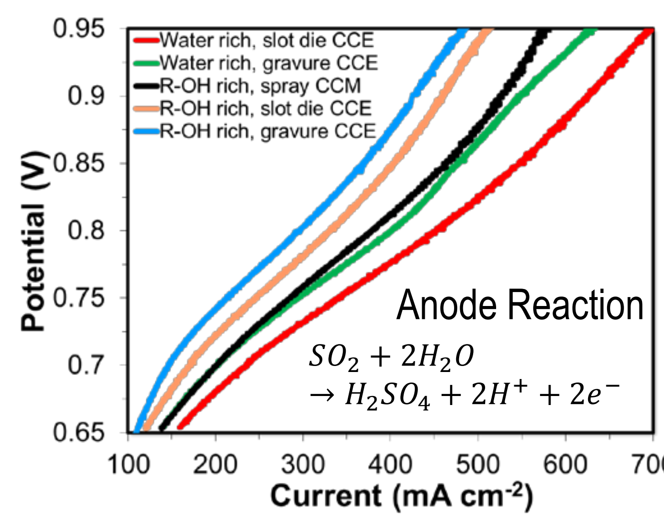
Correlating Half- and Single- LTE Cells Similar Ionomer Content Effect





- Ionomer content has a similar effect on MEA and half-cell performance
- Ionomer balance is needed for optimal performance

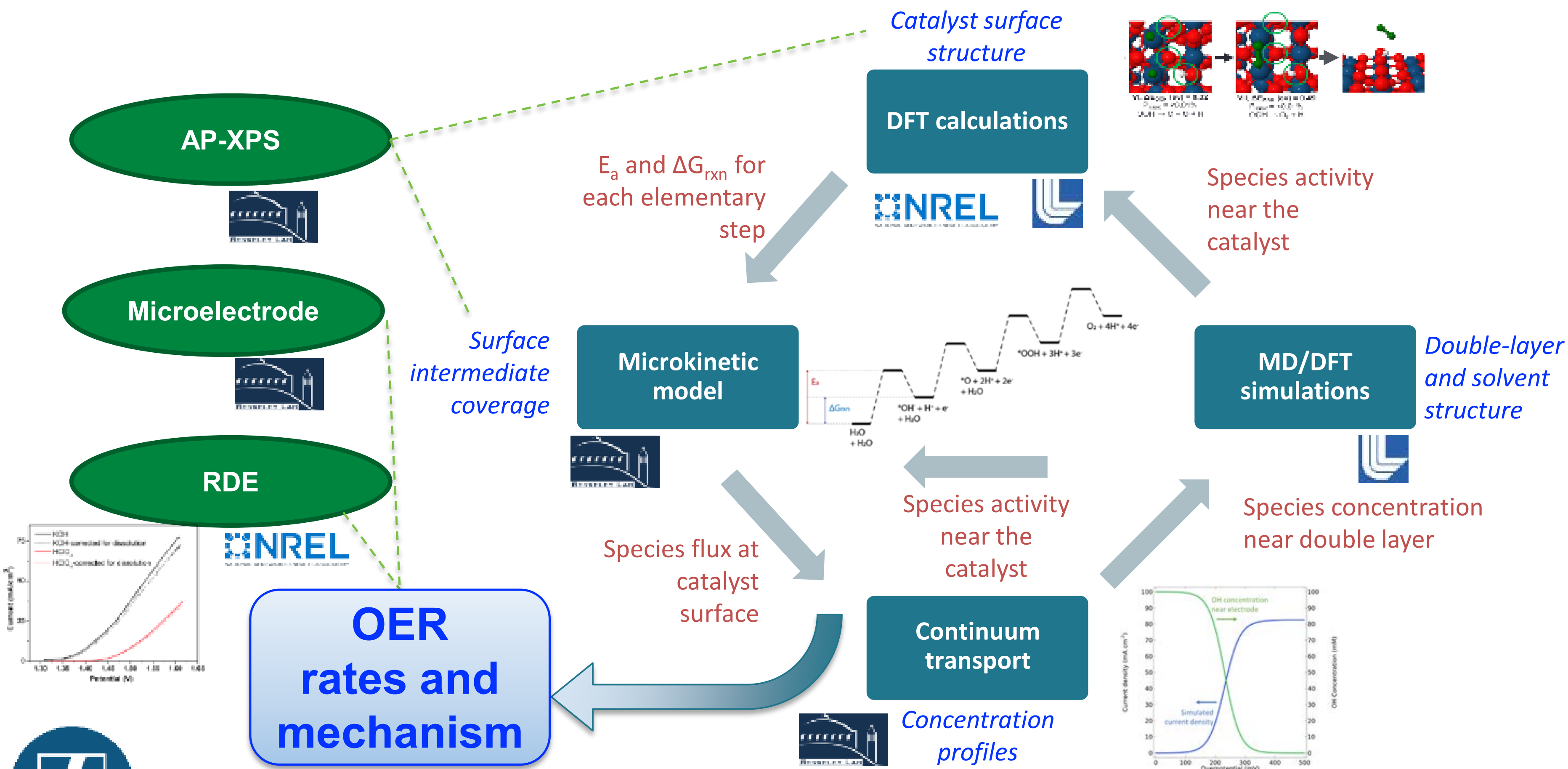
Ink Formulation and Electrode Processing Affect SO_2 Electrolysis Performance



- Material exchange between NREL and SRNL
- Water-rich inks and slot-die-made MEAs performed better than alcohol-rich (R-OH) inks and gravure-prepared MEAs.

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

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

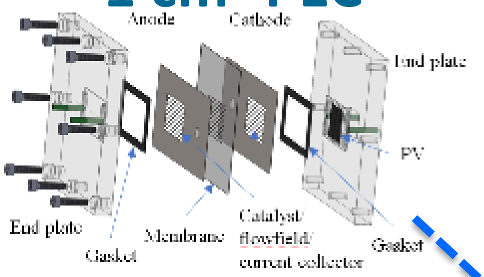


- *Developed various model handoff requirements and interactions*
  - *Microkinetic model for OER pathways formulated*
  - *Initial barriers for OER on IrO_2 in acid calculated*
- *Experimental characterization of OER on IrO_2 (RDE, AP-XPS, ME) initiated*

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

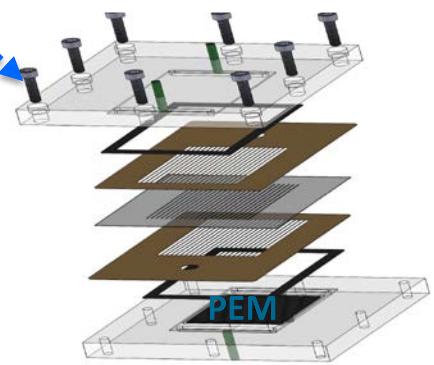
***Goal**: Understand integration issues and emergent degradation mechanisms of PEC devices at relevant scale, and demonstrate an integrated and durable 50 cm^2 PEC panel.*

1 cm^2 PEC



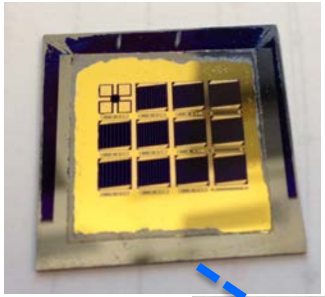
4 cm^2 PEC

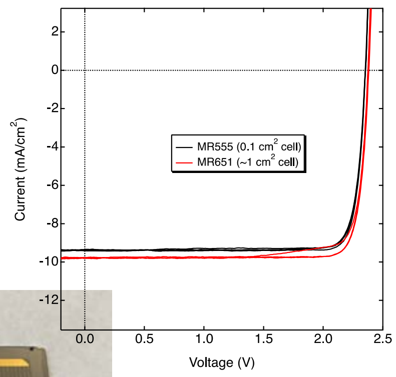
Anode Flowfield/GDL



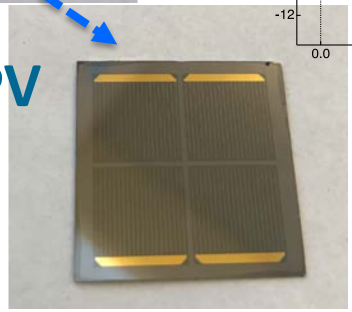
Cathode Flowfield/GDL

0.1 cm^2 PV





1 cm^2 PV



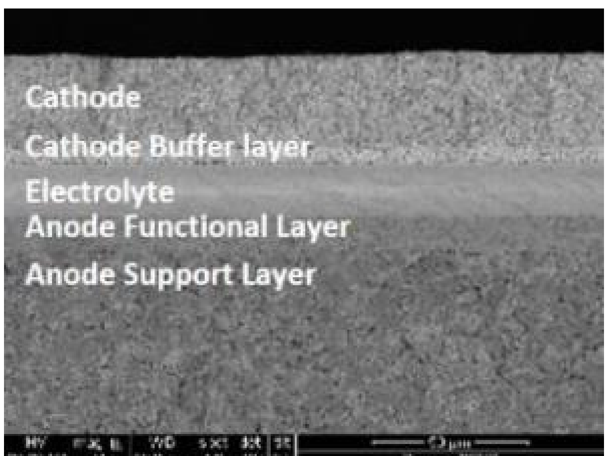
***Accomplishments**: PV fabrication scale up from 0.1 to 1 cm^2*
PEC vapor cell scale up from 1 to 4 cm^2
Benchmarking PEC cell performance between NREL and LBNL

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.*

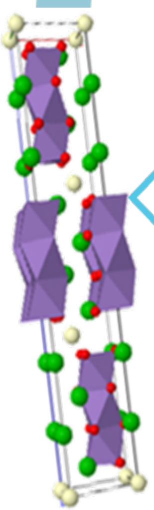
Accomplishments:

- ✓ First batch of YSZ-based SOEC fabricated using high-purity precursors.
- ✓ Sintering aid used in cathode buffer layers.
- ✓ Electrolyte thickness: 10-15 um.

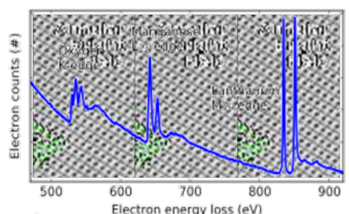


STCH Supernode: Develop Fundamental Understanding of the Mn-O Ligand Field's Influence on Water Splitting (LLNL, NREL, SNL; 6 Nodes)

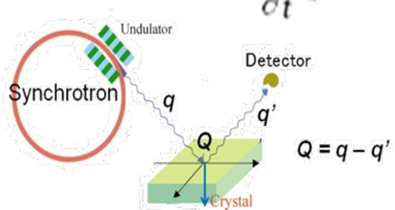
***Goal**: Develop a fundamental understanding of how unique electronic structures, induced by Mn-O ligand bond arrangements, influence favorable water-splitting material behavior.*

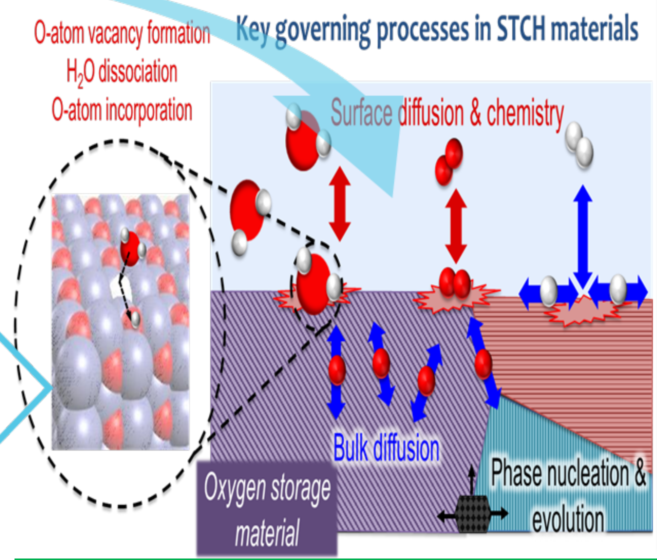


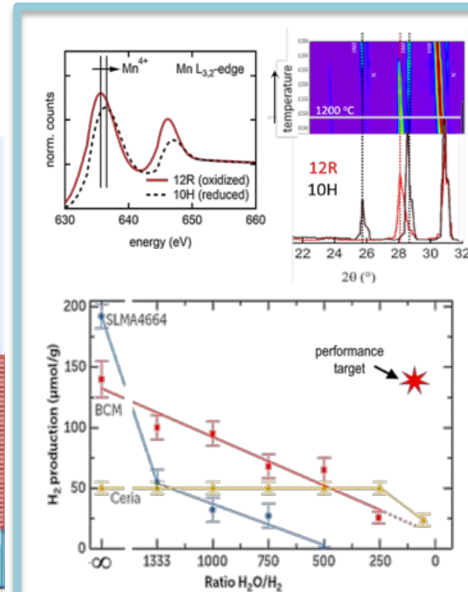
operando probes of Mn-O electronic structure



$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]\Psi = i\hbar\frac{\partial}{\partial t}\Psi$$







Accomplishments:

- *Develop synthetic routes to "ideal" Mn-O compounds*
- *Develop DFT methods to model core-hole spectroscopies*
- *Deploy operando test cell at SLAC (X-ray scattering)*
- *Conduct HR/STEM EELS studies on "ideal" compounds*

DFT = Density functional theory
HR/STEM EELS = high resolution/scanning transmission electron microscopy electron energy loss spectroscopy

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

Accomplishments:

- 1st Annual AWS community-wide benchmarking meeting (ASU, Oct. 24–25, 2018)
- 4 test frameworks developed
- 4 AWS technology surveys and result summaries published on the Data Hub
- 4 preliminary AWS roadmaps developed
- 1st round of test protocols defined and written
- Quarterly newsletters disseminated to AWS community
- >80 EMN capability nodes assessed; node gaps identified and communicated to HydroGEN

Goals:

- *Develop standardized best practices for characterizing and benchmarking AWSMs*
- *Foundation for accelerated materials RD&D for broader AWS community*
- *Extensive collaboration and engagement with HydroGEN steering committee, node subject matter experts, and broad water splitting community*

Development of Best Practices in Materials Characterization and Benchmarking: Critical to accelerate materials discovery and development

Responses to Previous Year Reviewers' Comments

- The fact that about half of the 80+ nodes (capabilities) are being utilized suggests that the interaction with the HydroGEN-supported R&D projects/community is a benefit toward helping DOE realize its goals. It is unclear how to put into perspective the number of users, page views, downloads, etc., as well as the publications and presentations, and whether these are helping DOE achieve its goals/targets. As HydroGEN "matures," a better metric would be clear evidence of how the nodes had an impact in making measurable/quantifiable benefits toward advancing R&D to meet DOE goals.

Response: We agree that testimonials and specific points of collaboration as witnessed by joint publications and presentations will be key in evaluating whether the nodes are providing critical or ancillary support for the FOA projects. Furthermore, cost reduction and technology maturity remain key metrics for success of the EMN.

- Probably one of the most pressing issues under Proposed Future Work is the development of an effective data management program, not so much in managing the data but in presenting to the R&D community in a format that is of value to the community. Developing benchmarking standard protocols and metrics is another pressing issue to make sure that the protocols for evaluating the various technologies provide an apples-to-apples comparison.

Response: We agree and are currently working on the data management in terms of dissemination with full metadata. In terms of protocols and metrics, this is an active area of work with the Benchmarking team lead by NEL/Proton OnSite, where HydroGEN core labs are actively engaged in helping to evaluate and establish the protocols.

Responses to Previous Year Reviewers' Comments

- Some of the secondary, visible metrics, such as the use of the data hub (~250 data files in a year), should get more emphasis either on boosting participation or in communicating the complexity of the data contained within the hub. There is ambiguity as to what a single file contains: whether it is a single resistance measurement or a summary from an entire collection of measurements from a unique tool on the beamline. In short, if the scale of the databank were conveyed in person-hours per data file that makes up the ~250 total, that could strike an audience as more impressive/appropriate than leaving the number of files to remain as an abstract concept, which risks sounding underwhelming.

Response: There has been lots of activities in the data hub this past year, hence there are 2 slides on data, summarizing the publication process developed, the various tools that have been developed, and the type of data that are on the data hub (e.g., microscopy, pol curves, XRD, XPS). Each data file represents one of these data. We hope these two slides better communicate the level of participation and the complexity of the data in the Data Hub.

- Although individual projects have milestones and go/no-go points, the AWSM Consortium lacks clear success metrics at a higher level to guide its pathways and projects.

Response: The success metrics for the consortium are varied. The overall metric is cost reduction (through performance and durability gains) for the various water-splitting materials, remaining cognizant that they are at very different levels of technological maturity. Interactions and enabling the FOA projects is key to this and thus serves as metrics for the consortium. In addition, the existence of supernodes (with their more traditional research metrics, shown on FY19 Supernode Annual Milestones [AM] slide in "Reviewers Only slides"), the data analysis and data hub, and the research progress of individual nodes all provide further metrics for measuring success.

Proposed Future Work

- Core labs will execute HydroGEN nodes to enable successful phase 2 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
- Collaborate and perform integrated research in the 5 supernodes
- Integrate whole system (capability nodes, FOA awardees, data infrastructure, TT/A) to accelerate the R&D of HydroGEN critical materials development to deployment
- Continue to review, maintain, and develop current and identify new relevant HydroGEN capability nodes
- 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
- Work closely with the Benchmarking Team to establish benchmarking, standard protocols, and metrics for the different water-splitting technologies
- Outreach

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

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

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

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

11 Labs **7** Companies **30** Universities **2** Funding Agencies

>80 unique, world-class capabilities/expertise:

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

- 16 projects successfully passed GNG
- 5 new Supernodes
- 4 new NSF DMREF projects
- 2 new HTE projects
- 2 Work for Others agreements
- 5 new data tools; >4,000 files
- 4 partner testimonial videos
- 1 annual benchmarking workshop
- Multiple AWS standard protocols

LTE Node Labs: INL Idaho National Laboratory, Berkeley Lab, NREL, Lawrence Livermore National Laboratory

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

LTE Projects: Proton OnSite / nel, Argonne National Laboratory, Northeastern University Center for Renewable Energy Technology, Los Alamos National Laboratory

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

Acknowledgements

Energy Materials Network
U.S. Department of Energy

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Advanced Water Splitting Materials

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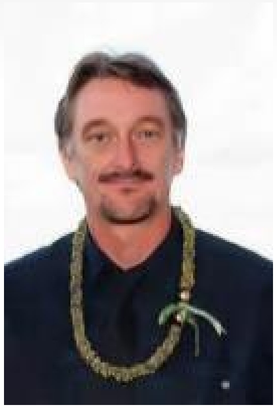

Eric Miller

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy
Fuel Cell Technologies Office

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Consultant: Karl Gross

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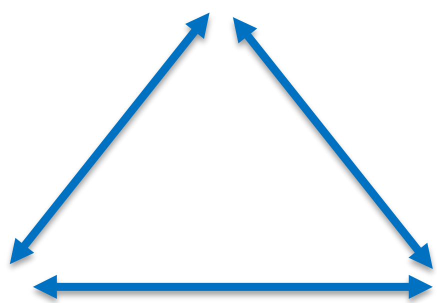

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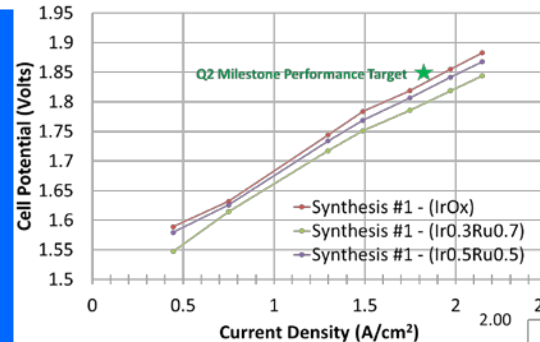
NREL – National Renewable Energy Laboratory | Berkeley Lab | Sandia National Laboratories | INL – Idaho National Laboratory | Lawrence Livermore National Laboratory | SRNL

Technical Backup Slides

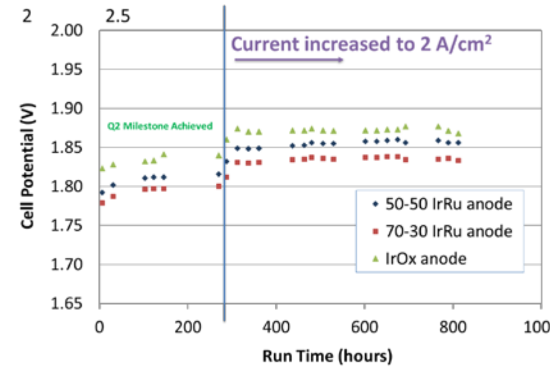
Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

Low Temperature Electrolysis (LTE)

NREL's contributed towards **Proton Onsite** achievement of **1.8 V at 2.0 A/cm²**, and **800 h PEM electrolysis durability at 2 A/cm²**, operating at 80°C and 30 bar. Proton's improved cell efficiency **is a step towards achieving its PEM water electrolysis cell efficiency goal of 43 kWh/kg** (1.7 V at 90°C) and at a cost of \$2/kg H_2, a significant improvement over the state-of-the-art cell efficiency of 53 kWh/kg.

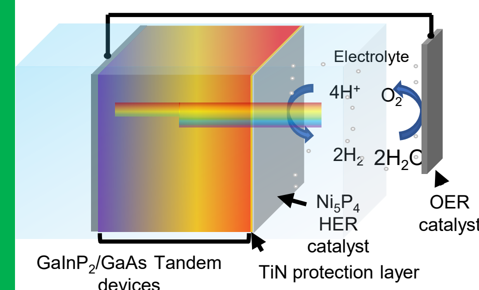


PROTON ON SITE
nel number one by nature
YOUR SOURCE FOR ALL THINGS HYDROGEN

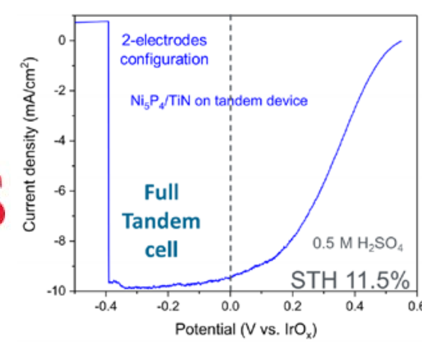


Photoelectrochemical (PEC) Water Splitting

NREL's high performance photoabsorber ($GaInP_2/GaAs$), integrated with **Rutgers' PGM-free electrocatalysts** ($LiCoO_2$ and Ni_5P_4) and protection layer (TiN), achieved a solar-to-hydrogen efficiency of **11.5%** for unassisted water splitting, on par performance with conventional PGM electrocatalysts (PtRu).



RUTGERS



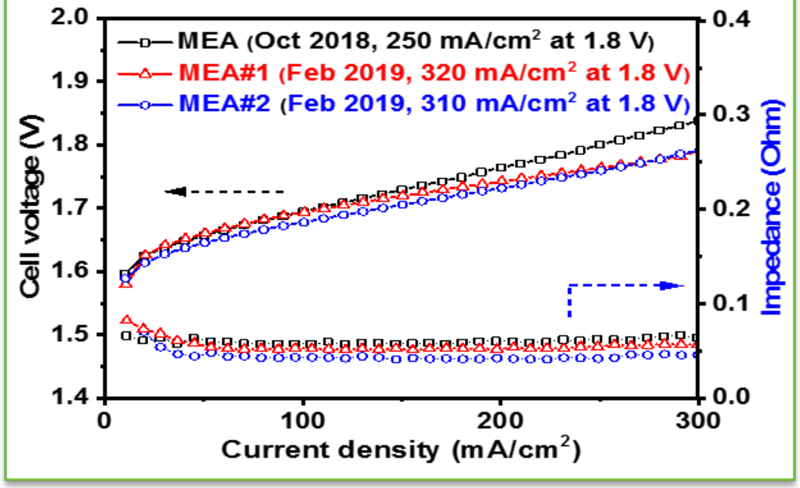
(NREL FY2018 Q4 AM – see Reviewer-Only slides)

Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

Low Temperature Electrolysis (LTE)

ANL demonstrated a **25 % improvement in PEM electrolysis cell performance** (310 mA/cm^2 at 1.8 V), using **PGM-free Co-ZIF derived OER** and Pt/C HER catalysts, N115 membrane, 60°C & 10 psi DI water, enabling the goal to reduce the anode catalyst cost by > 20 folds for the widespread implementation of PEME H_2 production. LBNL, LLNL, NREL, and SNL modeling, XPS, and microscopy nodes, respectively, contributed towards this achievement.

Argonne NATIONAL LABORATORY

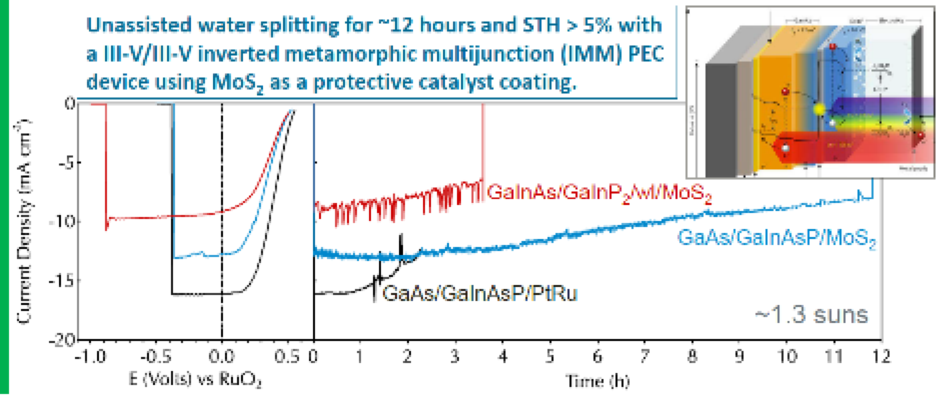


Photoelectrochemical (PEC) Water Splitting

SU demonstrated **unassisted PEC water-splitting** with **PGM-free MoS_2 HER catalyst** that achieved solar-to-hydrogen (**STH**) efficiency **> 5% under 1 sun,** providing a viable path for achieving low cost, stable and high (20%) STH PEC devices through earth-abundant protective catalysts, novel growth schemes, and new tandem III-V/Si system that has the potential to dramatically reduce H_2 production cost. The project leverages the NREL III-V fabrication, PEC characterization, corrosion, and on-sun testing expertise.

STANFORD UNIVERSITY

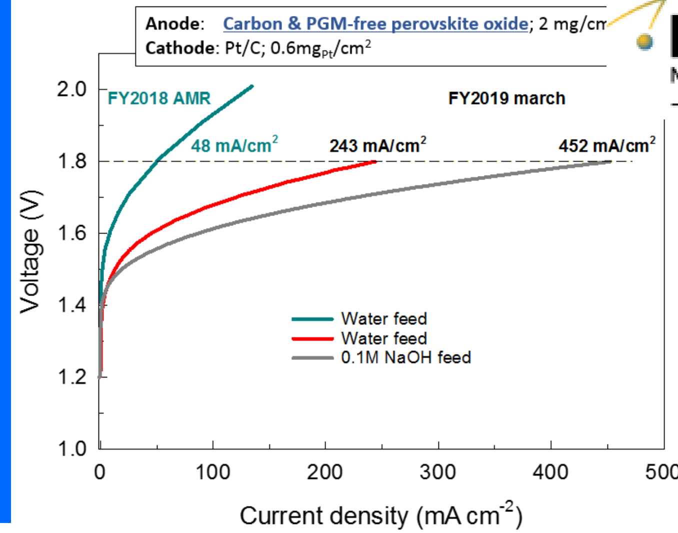
Unassisted water splitting for ~12 hours and STH > 5% with a III-V/III-V inverted metamorphic multijunction (IMM) PEC device using MoS_2 as a protective catalyst coating.



Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

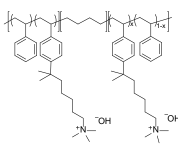
Low Temperature Electrolysis (LTE)

LANL demonstrated **4x higher** in **water-fed AEM electrolyzer performance (0.243 A/cm² at 1.8 V),** compared to FY2018, using LANL developed **carbon-free and PGM-free perovskite OER catalyst** and SNL AEM membrane. The goal is to achieve low cost H_2 production via high performing, durable, and low cost PGM-free catalyst AEM electrolysis. NREL XPS and in-situ testing nodes helped LANL understand the OER catalyst surface composition and MEA electrode performance.



Low Temperature Electrolysis (LTE)

LANL and RPI **prepared semi-crystalline AEM** membranes, by acid catalyzed polymerization & without using expensive metal catalyst, **that exceeded all of the project's (and state-of-the-art) membrane conductivity, alkaline stability, and mechanical strength targets,** as validated by LBNL characterization and modeling nodes. The goal is to synthesize and demonstrate high performing, durable, and economically-affordable AEMs in **water-fed AEM electrolysis**.



Properties
IEC = 1.71 mequiv./g
Water uptake = 144 %
In-plane swelling = 30%

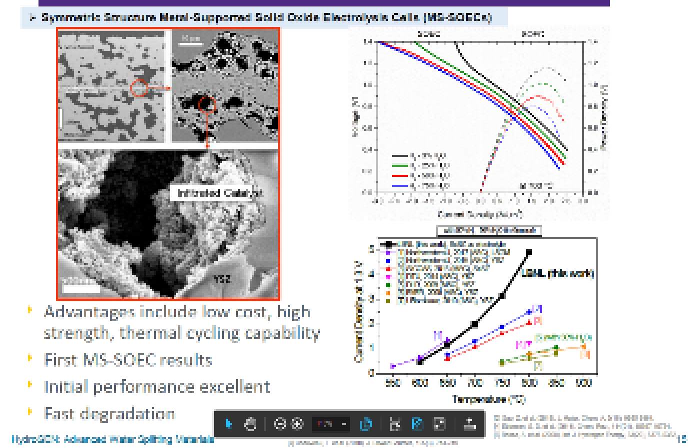
Properties	Target	Status
Hydroxide conductivity (mS cm^{-1}) at 30 °C	40	42 (30 °C) 54 (60 °C) 63 (80 °C)
Alkaline stability after 300 h in 1 M NaOH at 80 °C	< 5 % loss conductivity	0% loss
Mechanical toughness (mechanical strength (MPa) × % elongation) at 50 °C, 90% RH	> 1400	2091

Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

High Temperature Electrolysis (HTE)

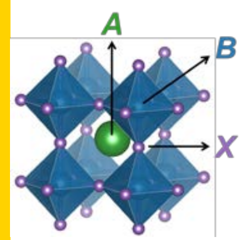
Using Northwestern University catalyst, YSZ electrolyte ($(ZrO_2)_{0.92}(Y_2O_3)_{0.08}$), and LBNL Metal-Supported Solid Oxide Cell and INL Advanced HTE testing nodes, the collaboration **demonstrated a metal-supported SOEC for the first time in electrolysis mode, with the highest performance** for oxygen-conducting type electrolysis cells to-date and promising stability.

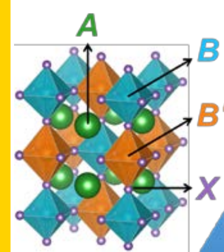
Northwestern

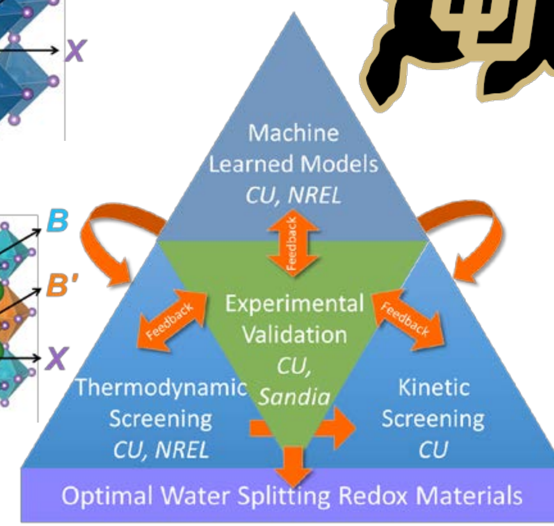


Solar Thermochemical (STCH) Water Splitting

The University of Colorado Boulder, with NREL's DFT node, developed and applied machine learning (ML) to accelerate STCH materials discovery, **identifying several hundred stable STCH perovskites** from over 1.1 million possible candidates, with **92% accuracy**. SNL's stagnation flow reactor and High-Temperature XRD nodes were used to **experimentally validate** water splitting kinetics and crystal structures for a select number of materials, providing critical feedback to **develop rapid kinetic screening techniques of materials**. Four materials have also been demonstrated to have H_2 productions **>200 µmol/g/cycle** at T_{red} =1450°C and ΔT=250°C, and results compared to computational predictions.



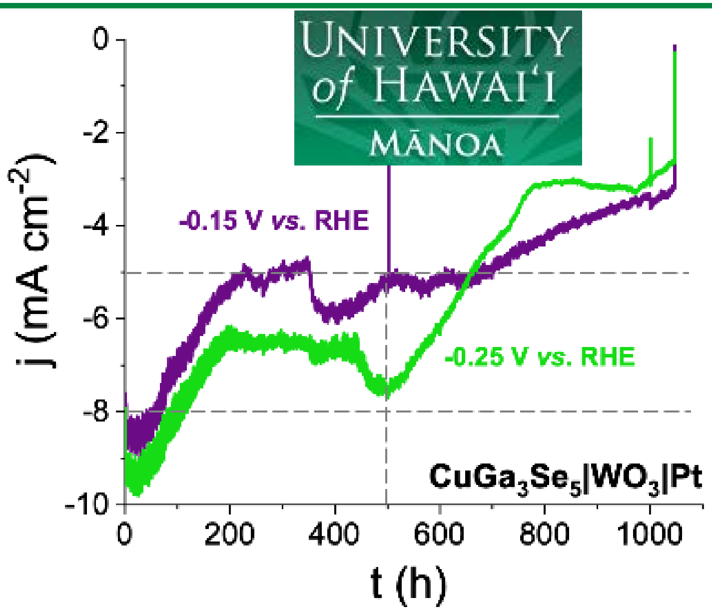




Accomplishments/Collaborations: HydroGEN Collaborative R&D Technical Highlights

Photoelectrochemical (PEC) Water Splitting

UH improved chalcopyrite stability in aqueous electrolyte by demonstrating **> 500 h of continuous operation at > 5 mA/cm²,** using a thin WO_3 coating on a high bandgap copper chalcopyrite, 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 STH efficiency > 10%. This project is supported by NREL synthesis and advanced characterization and LLNL modeling expertise to accelerate the development of materials and interfaces.



NSF-DMREF / DOE EERE HydroGEN EMN Example:

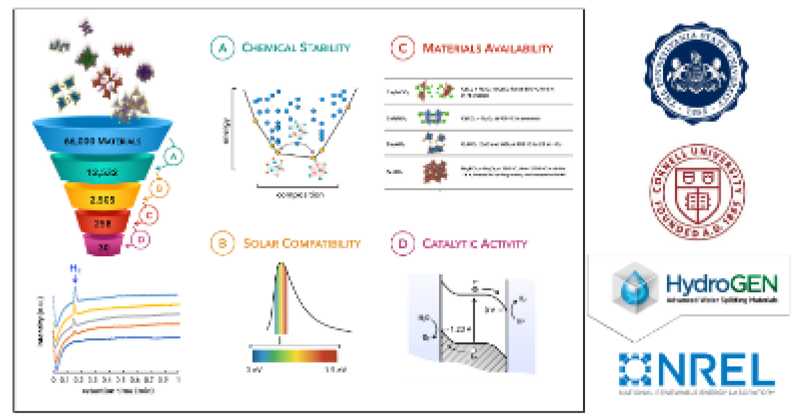
Photoelectrochemical (PEC) Water Splitting

Screening of photocatalysts for sustainable hydrogen generation

H. D. Abruña[1], I. Dabo[2], T. G. Deutsch[3], C. J. Fennie[1], V. Gopalan[2], R. E. Schaak[2]

[1]Cornell University [2]The Pennsylvania State University [3]National Renewable Energy Laboratory

Award DMREF-1729338



Starting from 66,000 materials from the *Materials Project*, 30 candidate photocatalysts have been screened by computing their chemical stability, solar compatibility, and catalytic activity. The ability to synthesize these materials is ensured by a systematic survey of the literature. Experiment shows hydrogen generation for four of the nine candidates tested so far.

Reviewer-Only Slides

FY19 NREL AOP Milestones

Milestone Name/Description	End Date	Type	Status
Kick-start the three NSF DMREF projects that NREL is supporting (PSU PEC, PSU LTE, and CSM STCH) and integrate them into HydroGEN.	12/31/2018	Q1 QPM	**Complete**
Initiate the 5 supernode efforts including a joint virtual kick-off meeting for each one. (NREL, LBNL, SNL, LLNL, INL, SRNL).	3/31/2019	Q2 QPM	**Complete**
Integrate new services into the Data Hub, including centralized authorization and sample management functions. Much of the HydroGEN research hinges on aligning and associating characterization and modeling data to uniquely identified samples. We will implement a sample management service into the Data Hub, which will include a backend database, an API layer and a data security layer. For centralized authorization, we will implement the Cognito Authentication service into the Data Hub, enabling 2-factor authentication consistently across all EMN data hubs.	6/30/2019	Q3 QPM	**On Track (central authorization is complete)**
Quantify the relationship between the exchange current density, specific activity and electrochemical surface area of a standard LTE OER catalyst via RDE with in-situ performance for at least 3 different electrode processing conditions and/or compositions, with properties comparable to IrO_2 (mass exchange current density = 0.075 mA/mg, ECA = 28.7 m^2/g and specific exchange current density = 0.26 μA/cm^2). (LTE/Hybrid Supernode Milestone)	9/30/2019	Q4 Annual Milestone	**On Track**

FY19 Supernode Annual Milestones (AM)

Milestone Name/Description	Supernode/ Lab AOP	Type	Status
Compare the exchange current density, specific activity and electrochemical surface area of a standard Hybrid Sulfur Cycle anode electro-catalyst via RDE with in-situ performance for at least 3 different electrode processing conditions and/or compositions with the goal of approaching 50-60% agreement between ex-situ and in-situ test.	LTE/Hybrid SRNL	Q4 AM 9/30/2019	**On Track**
Multiscale model predicts dominant reaction pathway with overall reaction rates in agreement within 10% error with experimental data for OER on IrO_2 under acidic conditions at two different applied overpotentials.	OER LBNL & LLNL	Q4 AM 9/30/2019	**On Track**
The synthesized microstructures of 4-6 electrode/electrolyte pure phase material will be analyzed to confirm repeatability of microstructure and composition via microscopy and X-ray diffraction analysis. The materials will have no secondary phases and the microstructure will have porosity and pore size within 10% of each other.	HTE INL	Q4 AM 9/30/2019	**On Track**
Identify one or more Mn-O baseline systems sharing key characteristics with BCM, which produces 3x more hydrogen than CeO2 when reduced at 1350°C and maintains higher water splitting favorability than SLMA at low oxygen partial pressure (>50 umole/g at H2O/H2 ratio<500). Data from SNL nodes will support first principles model development and refinement activities.	STCH SNL	Q4 AM 9/30/2019	**On Track**
Measure efficiency and durability a device of 8 cm2 or larger area using a flexible-platform photoreactor equipped with multiple in-situ diagnostic techniques on 2-axis tractor for 2+ days.	PEC LBNL & NREL (not in AOP)	Q4 AM 9/30/2019	**On Track**

FY18 AOP Milestones

Milestone Name/Description	End Date	Type	Status
Organize and host a HydroGEN project kick-off meeting for the 19 new FOA awardees and the 6 core lab members to help integrate them into the EMN.	12/31/2017	QPM	Complete Nov. 2017
80 HydroGEN capabilities reviewed based on developed process and evaluation criteria (e.g., utilization across the 18 new FOA projects).	3/30/2018	Annual Milestone	Complete
Integrate a data publication process into the data hub, enabling methods for assigning DOIs to uniquely identify public datasets and processes for approving and sharing data with the public.	6/30/2018	QPM	Complete (slide 10)
Benchmark solar-to-hydrogen efficiency of best-in-class LiCoO2 anode and Ni5P4 cathode catalysts integrated on an upright GaInP2/GaAs tandem cell with a target of greater than 10%.	9/30/2018	QPM	Complete (slide 39)

Patents and Patent Applications

1. "Nanofiber Electrocatalyst," Di-Jia Liu and Lina Chong, US Patent Application Publication, US2019/0060888A1.
2. "Electrochemical cells for hydrogen gas production and electricity generation, and related structures, apparatuses, systems, and methods," Dong Ding, Hanping Ding, Wei Wu and Chaojiang. US Provisional Patent Application 62/751, 969 (2018).
3. "Electrochemical cells for hydrogen gas production and electricity generation, and related structures, apparatuses, systems, and methods," Dong Ding, Hanping Ding, Wei Wu and Chaojiang. US Provisional Patent Application 62/722, 151 (2018).

Publications

1. S.M. Alia and G.C. Anderson. “Iridium Oxygen Evolution Activity and Durability Baselines in Rotating Disk Electrode Half-Cells.” *Journal of The Electrochemical Society* 166, no. 4 (2019): F282–294.
2. S.M. Alia and B.S. Pivovar. “Evaluating Hydrogen Evolution and Oxidation in Alkaline Media to Establish Baselines.” *Journal of The Electrochemical Society* 165, no. 7 (2018): F441–55. https://doi.org/10.1149/2.0361807jes.
3. T.A. Kistler, D. Larson, K. Walczak, P. Agbo, I.D. Sharp, A.Z. Weber, and N. Danilovic. “Integrated Membrane-Electrode-Assembly Photoelectrochemical Cell under Various Feed Conditions for Solar Water Splitting.” *Journal of The Electrochemical Society* 166, no. 5 (2019): H3020–28. https://doi.org/10.1149/2.0041905jes.
4. C.P. Muzzillo, W.E. Klein, Z. Li, A.D. DeAngelis, K. Horsley, K. Zhu, and N. Gaillard. “Low-Cost, Efficient, and Durable H2 Production by Photoelectrochemical Water Splitting with CuGa3Se5 Photocathodes.” *ACS Applied Materials & Interfaces* 10, no. 23 (2018): 19573–79. https://doi.org/10.1021/acsami.8b01447.
5. T.R. Hellstern, D.W. Palm, J. Carter, A.D DeAngelis, K. Horsley, L. Weinhardt, W. Yang, M. Blum, N. Gaillard, C. Heske, and T.F Jaramillo. “Molybdenum Disulfide Catalytic Coatings via Atomic Layer Deposition for Solar Hydrogen Production from Copper Gallium Diselenide Photocathodes.” *ACS Appl. Energy Mater.* 2, no. 2 (2019): 1060.
6. A.D. Deangelis, K. Horsley, and N. Gaillard. “Wide Band Gap $CuGa(S,Se)_2$ Thin Films on Transparent Conductive Fluorinated Tin Oxide Substrates as Photocathode Candidates for Tandem Water Splitting Devices.” *The Journal of Physical Chemistry C* 122, no. 26 (2018): 14304.

Publications

7. S. Hwang, S.H. Porter, A.B. Laursen, H. Yang, M. Li, V. Manichev, K.U.D. Calvinho, V. Amarasinghe, M. Greenblatt, E. Garfunkel, and G.C. Dismukes. “Creating stable interfaces between reactive materials: Titanium nitride protects photoabsorber-catalyst interface in water-splitting photocathodes.” *J. Mater. Chem. A* 7 (2019): 2400–2411.
8. D. Arifin and A.W. Weimer. “Kinetics and Mechanism of Solar-thermochemical H2 and CO Production by Oxidation of Reduced CeO2.” *Solar Energy* 160 (2018): 178–185. https://doi.org/10.1016/j.solener.2017.11.075.
9. E. Liu, L. Jiao, H. Doan, Z. Liu, Y. Huang, K.M. Abraham, and S. Mukerjee. “Unifying Alkaline Hydrogen Evolution/Oxidation Reaction Kinetics by Identifying the Role of Hydroxy-Water-Cation Adducts.” *J. Amer. Chem. Soc.* 141 (2019): 3232–3239.
10. Q. Jia, E. Liu, L. Jiao, and S. Mukerjee. “Current Understanding of Sluggish Kinetics of Hydrogen Evolution and Oxidation reactions in Base.” *Current Opinion in Electrochemistry* (In Press).
11. J.Y. Jeon, S. Park, J. Han, S. Maurya, A.D. Mohanty, D. Tian, N. Saikia, M.A. Hickner, C.Y. Ryu, M.E. Tuckerman, S.J. Paddison, Y.S. Kim, and C. Bae. “Synthesis of Aromatic Anion Exchange Membranes by Friedel-Crafts Bromoalkylation and Cross-Linking of Polystyrene Block Copolymers.” *Macromolecules* (2019). https://doi.org/10.1021/acs.macromol.8b02355.
12. D. Li, I. Matanovic, A.S. Lee, E.J. Park, C. Fujimoto, H.T. Chung, and Y.S. Kim. “Phenyl Oxidation Impacts the Durability of Alkaline Membrane Water Electrolyzer,” *ACS Applied Materials and Interfaces* (2019). https://doi.org/10.1021/acsami.9b00711.

Publications

13. F.A. Chowdhury, M.L. Trudeau, H. Guo and Z. Mi. "A Photochemical Diode Artificial Photosynthesis System for Unassisted High Efficiency Overall Pure Water Splitting." *Nature Communications* 9 (2018): 1707. https://doi.org/10.1038/s41467-018-04067DO.
14. W. Wu, H. Ding, Y. Zhang, Y. Ding, P. Katiyar, P. Majumdar, T. He, and D. Ding. "3D Self-Architectured Steam Electrode Enabled Efficient and Durable Hydrogen Production in A Proton Conducting Solid Oxide Electrolysis Cell at Temperatures Lower than 600^{o}C." *Advanced Science* 11 (2018): 1870166. Frontispiece Feature: https://onlinelibrary.wiley.com/doi/10.1002/advs.201870070.
15. R. Wang, C. Byrne, and M.C. Tucker. "Assessment of Co-Sintering as a Fabrication Approach for Metal-Supported Proton-Conducting Solid Oxide Cells." *Solid State Ionics* 332 (2019): 25–33.
16. S.-L. Zhang, H. Wang, M.Y. Lu, A.-P. Zhang, L.V. Mogni, Q. Liu, C.-X. Li, C.-J. Li, and S.A. Barnett. "Cobalt-substituted SrTi0.3Fe0.7O3: a stable high-performance oxygen electrode material for intermediate-temperature solid oxide electrochemical cells." *Energy and Environmental Science*, 11 (2018): 1870-1879. https://doi.org/10.1039/C8EE00449H.
17. D.R. Barcellos, M.D. Sanders, J. Tong, A.H. McDaniel, and R.P. O'Hayre. "BaCe0.25Mn0.75O3-δ — A Promising Perovskite-type Oxide for Solar Thermochemical Hydrogen Production." *Energy and Environmental Science* 11 (2018): 3256-3265. https://doi.org/10.1039/C8EE01989D.
18. H.N. Dinh, R. Boardman, A.H. McDaniel, H. Colon-Mercado, T. Ogitsu, A.Z. Weber. "HydroGEN Overview: A Consortium on Advanced Water Splitting Materials (AWSM)." FY 2018 DOE Hydrogen and Fuel Cells Program Annual Progress Report.

Publications

19. G.S. Gautam and E.A. Carter, "Evaluating transition metal oxides within DFT-SCAN and SCAN+U frameworks for solar thermochemical applications," *Phys. Rev. Mater.* 2 (2018): 095401.
20. C. Bartel, A. Weimer, S. Lany, C. Musgrave, and A. Holder, "The role of decomposition reactions in assessing first-principles predictions of solid stability," *npj Computational Materials* 5, no. 1 (2019): 4.
21. C. Bartel, C. Sutton, B. Goldsmith, R. Ouyang, C. Musgrave, L. Ghiringhelli, and M. Scheffler, "New tolerance factor to predict the stability of perovskite oxides and halides," *Science Advances* 5, no. 2 (2019): eaav0693.
22. C. Bartel, S. Millican, A. Deml, J. Rumptz, W. Tumas, A. Weimer, S. Lany, V. Stevanovic, C. Musgrave, and A. Holder, "Physical descriptor for the Gibbs energy of inorganic crystalline solids and temperature-dependent materials chemistry," *Nature Communications* 9, no. 1 (2018): 4168.
23. M. Carmo, C. Liu, G. Bender, A. Everwand, T. Lickert, T. Smolinka, D. Stolten, W. Lehnert, "Performance enhancement of PEM electrolyzers through Iridium-coated Titanium Porous Transport Layers," Electrochemistry Communications 97 (2018): 96–99, https://doi.org/10.1016/j.elecom.2018.10.021.
24. G. Bender, M. Carmo, T. Smolinka, A. Gago, N. Danilovic, M. Mueller, F. Ganci, A. Fallisch, P. Lettenmeier, K.A. Friedrich, K. Ayers, B. Pivovar, J. Mergel, D. Stolten, "Initial Approaches in Benchmarking and Round Robin Testing for Proton Exchange Membrane Water Electrolyzers," *International Journal of Hydrogen Energy* (accepted for publication).

Presentations

1. (**Invited**) H.N. Dinh, A.H. McDaniel, A.Z. Weber, R. Boardman, T. Ogitsu, H. Colon-Mercado, "HydroGEN: A Consortium on Advanced Water Splitting Materials," 9th IEA Annex 30 Electrolysis Workshop, NREL, Golden, CO, September 27, 2018.
2. (**Invited**) H.N. Dinh, A.H. McDaniel, A.Z. Weber, R. Boardman, T. Ogitsu, H. Colon-Mercado, "HydroGEN: A Consortium on Advanced Water Splitting Materials," HydroGEN AWS Technology Pathways Benchmarking & Protocols Workshop, Arizona State University, Tempe, AZ, October 24, 2018
3. (**Invited**) H.N. Dinh, "FCTO's HydroGEN AWSM Energy Materials Network Overview Webinar," DOE Fuel Cell Technologies Office Webinar, February 7, 2019.
4. (**Invited**) H.N. Dinh, K. Randolph, A.Z. Weber, A.H. McDaniel, R. Boardman, T. Ogitsu, D.L. Anton, D. Peterson, E.L. Miller, "HydroGEN Overview, Projects, and the AWSM Node Capabilities," Symposium ES11–Advanced Low Temperature Water Splitting for Renewable HydroGEN Production via Electrochemical and Photoelectrochemical Processes, Spring MRS Meeting, Phoenix, AZ, April 24, 2019.
5. (**Invited**) H.N. Dinh, D. Peterson, K. Randolph, A. Z. Weber, A.H. McDaniel, R. Boardman, T. Ogitsu, D.L. Anton, "HydroGEN Overview and AWSM Electrolysis Project Updates," 235th ECS Meeting, Dallas, TX, May 24, 2019.

Presentations

6. K.E. Ayers, C. Capuano, P. Mani, "High Efficiency PEM Electrolysis: Potential for H2@Scale," 234th ECS Meeting, Cancun, Mexico, October 2, 2018.
7. R. Wang, M. Tucker, "Development of High Performance Metal-Supported Solid Oxide Electrolysis Cells," 234th ECS Meeting (AiMES 2018), Cancun, Mexico, October 2018.
8. (**Invited**) S. Barnett, "High-Efficiency Electrical Energy Storage Using Reversible Solid Oxide Cells," Boston University Materials Day–Materials for Electrochemical Energy Conversion & Storage, Boston, MA, October 26, 2018.
9. (**Invited**) N. Gaillard, A.D. DeAngelis, K. Horsley, "Wide Bandgap Copper Chalcopyrite Candidates for Renewable Hydrogen Generation," 233rd ECS Meeting, Symposium I05, 1884, Seattle, WA, 2018.
10. (**Invited**) T. Ogitsu, J. Varley, A. Deangelis, K. Horsley, N. Gaillard, "Integrating Ab-Initio Simulations and Experimental Characterization Methods: Towards Accelerated Chalcopyrite Materials Development for Hydrogen Production," 233rd ECS Meeting, Symposium I05, 1855, Seattle, WA, 2018.
11. K. Horlsey, A. Deangelis, N. Gaillard, "Cu(In,Ga)S_2 Photocathodes with Optical Bandgap Over 1.7 eV for Photoelectrochemical Water Splitting," MRS Spring Meeting, Symposium EN18, EN18.15.05, Phoenix, AZ, 2018.
12. A. Deangelis, K. Horlsey, N. Gaillard, "Wide-Bandgap CuGa(S,Se)2 As Top Cell Photocathodes for Tandem Water Splitting Devices," 233rd ECS Meeting, Symposium I05, 1929, Seattle, WA, 2018.

Presentations

13. S. Mukerjee and J. Qingying, "Fundamental aspects of regenerative hydrogen electrocatalysis in alkaline pH." In *Abstracts of Papers of the American Chemical Society* 256 (2018).
14. I. Kendrick, M. Bates, Q. Jia, H. Doan, W. Liang, S. Mukerjee, "Tuning Ni Surfaces for Enhanced Oxygen Evolution Reaction." In *Meeting Abstracts* 29 (The Electrochemical Society, 2018): 1702–1702.
15. D. Li, I. Matanovic, A.S. Lee, E.J. Park, C. Fujimoto, H.T. Chung, Y.S. Kim, "Phenyl Oxidation at Oxygen Evolution Potentials," Polymers for Fuel Cells, Energy Storage and Conversion, Asilomar Conference Ground, Pacific Grove, CA, USA, Feb. 24–27, 2019.
16. E.J. Park, S. Maurya, M.R. Hibbs, C.H. Fujimoto, Y.S. Kim, "Caveat of High Temperature Accelerated Stability Test of Anion Exchange Membrane," Polymers for Fuel Cells, Energy Storage and Conversion, Asilomar Conference Ground, Pacific Grove, CA, USA, Feb. 24–27, 2019.
17. H.T. Chung, "Carbon-free Perovskite Oxide OER Catalysts for AEM Electrolyzer," Abstract number IO3-1687, 233rd ECS Meeting, Seattle, WA, May 13–17, 2018.
18. (**Invited**) L. Chong, H. Wang, D.-J. Liu, "PGM-free OER Catalysts for PEM Electrolyzer Application," 235th ECS Meeting, Dallas, TX, May 26–31, 2019.
19. A.S. Lee, Y.S. Kim, P. Zelenay, C. Fujimoto, L.-W. Wang, G. Teeter, G. Bender, D.-J. Liu, G. Wu, H. Xu, "PGM-free OER Catalysts for PEM Electrolyzer," Hydrogen Production Tech Team Meeting, Berkeley, CA, April 10, 2018.

Presentations

20. G.C. Dismukes, “Bioinspired heterogeneous electrocatalysts for CO2 reduction and water splitting: Energy-efficient C-C coupling rivaling enzymes,” Leiden University, Institute of Chemistry, Leiden, the Netherlands, Danish Technical University, Institute of Physics, Copenhagen, DK, Aarhus University, iNano, Aarhus, DK, October 2018.
21. E. Garfunkel, “Photoelectrochemical water splitting to form hydrogen,” 2018 Telluride Semiconductor Surface Chemistry Meeting, Telluride CO.
22. X. (Jessica) Luo, A. Kusoglu, “Structure-Transport Relationships of Anion Exchange Ionomers,” ACS Division of Polymer Chemistry, Pacific Grove, CA, 2019 (Poster).
23. A.Z. Weber, “Exploring Polymer-Electrolyte Fuel Cells using Physics-Based Modeling,” Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany, December 2018.
24. J.C. Fornaciari, J. Zhou, D. Primc, A.T. Bell, A.Z. Weber, “Electrocatalyst performance for selective methanol formation in methane electrolyzer,” ECS Fall Meeting, Cancun, Mexico (poster).
25. R. Wang, C. Byrne, M.C. Tucker, “Proton-Conducting Ceramics for Metal-Supported Solid Oxide Cells,” 19th International Conference on Solid State Protonic Conductors, Stowe, VT, Sept. 21, 2018.
26. D. Ding, W. Wu, H. Ding, T. He, “Development of Proton-Conducting Solid Oxide Electrolysis Cells at Intermediate Temperatures at Idaho National Laboratory,” 234th ECS Meeting (AiMES 2018), Cancun, Mexico, Sept. 30–Oct. 4, 2018.

Presentations

27. D. Ding. "Development of Electrochemical Processing and Electrocatalysis at Intermediate Temperatures at Idaho National Laboratory (INL)," Invited Lecture for faculty and graduate students, Department of Mechanical and Aerospace, West Virginia University, Morgantown, WV, USA, Dec. 4, 2018.
28. B. Hu, M. Reisert, A. Aphale, S. Belko, O. Marina, J. Stevenson, D. Ding, P. Singh, "Barium Zirconate Based Electrolyte Densification Using Reactive Sintering Aids," 43rd International Conference and Exposition on Advanced Ceramics and Composites (ICACC 2019), Daytona Beach, FL, USA, Jan 27–Feb 1, 2019.
29. H. Ding, W. Wu, D. Ding, "A Novel Triple Conducting Electrode for Fast Hydrogen Production in Protonic Ceramic Electrochemical Cells (H-SOECs)." 43rd International Conference and Exposition on Advanced Ceramics and Composites (ICACC 2019), Daytona Beach, FL, USA, Jan 27–Feb 1, 2019.
30. D. Ding, "Advancement of Intermediate Temperature Solid Oxide Energy Conversion Technologies at Idaho National Laboratory." Invited Lecture for faculty and graduate students, Department of Chemical Engineering, University of Louisiana at Lafayette, Lafayette, LA, USA, April 1, 2019.
31. B. Hu, O.A. Marina, A.N. Aphale, D. Ding, H. Ding, A. Zakutayev, J. Stevenson, P. Singh, "Stable Proton-conducting Solid Oxide Electrolysis Cells for Pure Hydrogen Production at Intermediate Temperatures," 2019 MRS Spring Symposia on Advanced Water Splitting, Phoenix, AZ, April 22–26, 2019.

Presentations

32. D. Ding, "Advancement of reversible proton-conducting solid oxide cells at Idaho National Laboratory (INL)," 2nd International Conference on Electrolysis (ICE 2019), Loen, Norway, June 9–13, 2019.
33. C. Musgrave, C. Bartel, A. Holder, C. Sutton, B. Goldsmith, R. Ouyang, L. Ghiringhelli, M. Scheffler, "Ab Initio and Machine Learned Modeling for the Design and Discovery of New Materials for Energy Applications," Air Force Research Laboratories, Dayton, OH, January 2019.
34. S. Millican, I. Androschuk, A. Weimer, C. Musgrave, "Computational discovery of materials for solar thermochemical hydrogen production" American Institute of Chemical Engineers, October 2018.
35. C. Bartel, C. Sutton, B. Goldsmith, R. Ouyang, C. Musgrave, L. Ghiringhelli, M. Scheffler, "New tolerance factor to predict the stability of perovskite oxides and halides," American Institute of Chemical Engineers, October 2018.
36. C. Bartel, C. Sutton, B. Goldsmith, R. Ouyang, C. Musgrave, L. Ghiringhelli, M. Scheffler, "New tolerance factor to predict the stability of perovskite oxides and halides," European Materials Research Society, September 2018.
37. S. Millican, I. Androschuk, A. Weimer, C. Musgrave. "Rapid Kinetic Profiling of Bulk Diffusion Barriers for Solar Thermal Water Splitting Materials," 21st International Conference on Ternary and Multinary Compounds, September 2018.

Presentations

38. C. Bartel, C. Sutton, B. Goldsmith, R. Ouyang, C. Musgrave, L. Ghiringhelli, M. Scheffler, “New tolerance factor to predict the stability of perovskite oxides and halides,” 21st International Conference on Ternary and Multinary Compounds, September 2018.
39. C. Bartel, C. Sutton, B. Goldsmith, R. Ouyang, C. Musgrave, L. Ghiringhelli, M. Scheffler, “New tolerance factor to predict the stability of perovskite oxides and halides,” Application of Machine Learning and Data Analytics for Energy Materials Network Consortia 2018, May 2018.
40. S.L. Millican, I. Androshchuk, A.W. Weimer, C.B. Musgrave, “Ab-initio Modeling and Experimental Demonstration of Metal Oxides for Solar Thermochemical Water Splitting,” American Chemical Society Spring Meeting, March 2018.
41. C. Bartel, C. Sutton, B. Goldsmith, R. Ouyang, C. Musgrave, L. Ghiringhelli, M. Scheffler, “Improved tolerance factor for classifying the formability of perovskite oxides and halides,” American Physical Society Annual Meeting, March 2018.
42. C. Bartel, S. Millican, A. Deml, J. Rumptz, W. Tumas, A. Weimer, S. Lany, V. Stevanovic, C. Musgrave, A. Holder, “Machine learning the Gibbs energies of inorganic crystalline solids,” American Physical Society Annual Meeting, March 2018.
43. Millican, S.L., I. Androshchuk, A.W. Weimer, and C.B. Musgrave, “Design and Discovery of Mixed Metal Oxides for Solar Thermochemical Water Splitting,” International Conference and Exposition on Advanced Ceramics and Composites, January 2018.

Presentations

44. G. Bender, M. Carmo, S. Fischer, T. Lickert, T. Smolinka, J. Young, "IEA Annex 30 Overview," Invited talk at Proton 2B Workshop: HydroGEN Benchmarking & Protocols Workshop, October 24, 2018, Tempe Arizona.
45. J.L. Young, F. Ganci, S. Madachy, S. Fischer, M. Carmo, G. Bender, "PEM Electrolyzer Characterization and Limitations When Using Carbon-Based Hardware and Material Sets," Accepted ECS talk, 235th ECS Meeting, Dallas, TX, USA, May 26-31, 2019.
46. G. Bender, M. Carmo, S. Fischer, T. Lickert, T. Smolinka, J. Young, "Round Robin Testing for Polymer Electrolyte Membrane Water Electrolysis - Phase 2," World Hydrogen Energy Conference, Rio de Janeiro, June 19, 2018.
47. G. Bender, H.N. Dinh, N. Danilovic, A. Weber, "HydroGEN: Low-Temperature Electrolysis," Hydrogen and Fuel Cells Program 2018 AMR, Washington, DC, June 13, 2018.
48. J. Young, A. Kallen, E. Klein, S. Alia, G. Bender, "IEA Annex 30 Workshop – NREL LTE Activities Overview," Invited Talk, IEA Annex 30 Workshop, September 2018, Golden, Colorado, USA.
49. K. Ayers, A. Motz, C. Capuano, P. Mani, "Development of Protocols and Standards for Low Temperature Electrolysis," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
50. C. Xiang, "Development of Protocols and Standards for Photoelectrochemical Water-Splitting," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.

Presentations

51. O. Marina, “Framework and Test Protocols for High Temperature Electrolysis,” Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
52. E. Stechel, “Framework and Test Protocols for Solar Thermochemical Water Splitting,” Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
53. G. Dismukes, A.B. Laursen, S. Hwang, E. Garfunkel, T. Deutsch, D. Friedman, M. Steiner, “Electrochemical and Photoelectrochemical Water Splitting Using Bioinspired Catalysts That Out-Perform Nobel Metals,” Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
54. N. Danilovic, F. Houle, A. Kusoglu, F.M. Toma, M. Tucker, L.-W. Wang, A. Weber, “Low and High -Temperature Electrolysis, Photoelectrochemical and Solar Thermochemical Water Splitting Materials Characterization and Development at Berkeley Lab Under the HydroGEN Consortium,” Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
55. I. Khan, K. Heinselman, C. Muzzillo, J. Young, T. Deutsch, A. Zakutayev, N. Gaillard, “CuGa3Se5/Zn1-xMgxO Photocathodes for Photoelectrochemical Water Splitting,” Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
56. T. Jaramillo, “Development of Catalytic Coatings for H2-Producing Photocathodes in Solar Water-Splitting,” Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.

Presentations

57. N. Gaillard, "Wide Bandgap Chalcopyrites for Photoelectrochemical Water Splitting," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
58. J. Young, H. Doescher, J. Geisz, J. Turner, T. Deutsch, "Solar-to-Hydrogen Efficiency—Shining Light on Photoelectrochemical Device Performance," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
59. T. Deutsch, J. Young, C. Aldridge, C. Barraugh, M. Steiner, "Photoelectrochemical Water Splitting Durability Testing—What Can Half-Cell Results Can Tell Us About Full-Cell Performance?" Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
60. W. Drisdell, A. Landers, M. Farmand, "Operando Synchrotron Characterization of Electrochemical Interfaces," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
61. N. Danilovic, T. Kistler, S. Alia, P. Agbo, A. Weber, "Benchmarking Water-Splitting Materials at the Intersection of Electrocatalysis and Photoelectrochemistry," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
62. G. Bender, S. Alia, M. Ulsh, S. Mauger, B. Pivovar, H. Dinh, A. Weber, N. Danilovic, A. Kusoglu, H. Colon-Mercado, "HydroGEN Supernode—Linking Low Temperature Electrolysis (LTE)/Hybrid Materials to Electrode Properties to Performance," Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.

Presentations

63. J. Young, N. Danilovic, M. Steiner, F.M. Toma, G. Saur, J. Vidal, H. Breunig, D. Friedman, A. Weber, T. Deutsch, “HydroGEN PEC Supernode—Emergent Degradation Mechanisms with Integration and Scale Up of PEC Devices,” Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
64. T. Ogitsu, J. Varley, A. Sharan, A. Janotti, N. Gaillard, A. DeAngelis, “Chalcopyrite Alloy Materials for PEC H2 Production—Development of Theoretical Synthesis Support System for HydroGEN,” Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
65. T. Ogitsu, B. Wood, T.A. Pham, J. Varley, J. Lee, M. Biener, C. Orme, Y. Han, “Photoelectrochemical and Low Temperature Water Splitting Materials Research at Lawrence Livermore National Laboratory Under HydroGEN Consortium,” Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
66. R. Bell, D. Ginley, P. Parilla, S. Lany, E. Coker, A. Zakutayev, A. McDaniel, “Design, Synthesis, and Characterization of High Quality STCH Materials,” Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
67. A. McDaniel, A. Ambrosini, E. Coker, J. Sugar, R. Bell, D. Ginley, S. Lany, P. Parilla, T. Ogitsu, S. Wan, B. Wood, “Developing an Atomistic Understanding of the Layered Perovskite Ba4CeMn3O12 and Its Polytypes for Thermochemical Water Splitting—A HydroGEN Supernode,” Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.

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68. O. Marina, K. Meinhardt, G. Whyatt, D. Reed, K. Recknagle, B. Koeppel, J. Holladay, "High Temperature Electrolysis Capabilities at PNNL—Materials Development, Cell/Stack Manufacturing, Testing, Characterization and Modeling," Poster presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
69. M. Gerhardt, L. Stanislaw, A. Weber, "Modeling of Anion-Exchange Membrane Electrolyzers to Guide Materials Development," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
70. S. Alia, S. Ghoshal, G. Anderson, M.-A. Ha, S. Stariha, C. Ngo, S. Pylypenko, R. Borup, R. Larsen, "Effects of Low Loading and Intermittency on Low Temperature Electrolysis from a Catalyst Perspective," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
71. H. Xu, "Alkaline Membrane Electrolysis—Challenges and Perspectives," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
72. Z. Mi, S. Vanka, "Monolithically Integrated InGaN/Si Tandem Photoelectrodes for Efficient and Stable Photoelectrochemical Water Splitting," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
73. H. Lim, J. Young, J. Geisz, D. Friedman, T. Deutsch, J. Yoon, "Surface-Tailored GaInP2 Photocathodes for High Performance Solar Water Splitting," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.

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74. T.A. Pham, Z. Mi, T. Ogitsu, "Probing the Surface Chemistry and Stability of III-V Photoelectrodes with First-Principles Simulations and In Situ Experiments," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
75. C. Musgrave, C. Bartel, S. Millican, B. Goldsmith, C. Sutton, S. Lany, A. Weimer, A. Holder, "Ab Initio and Machine Learned Modeling to Screen and Discover Materials for Solar Thermal Water Splitting," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
76. R. Bell, P. Parilla, E. Coker, E. Stechel, D. Ginley, "Developing Standard Materials for Solar Thermochemical Water Splitting Calibration," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
77. R. Bell, X. Qian, E. Coker, M. Rodriguez, P. Parilla, S. Haile, D. Ginley, "In-Situ Defect Mapping of High Temperature STCH Materials in Oxidizing and Reducing Environments," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
78. R. O'Hayre, M. Sanders, D. Barcellos, C. Duan, J. Huang, M. Papac, V. Stevanovic, N. Kumar, A. Zakutayev, S. Lany, A. Emery, C. Wolverton, C. Borg, A. McDaniel, "The 'Perovskite Playground'—Engineering Defect Chemistry in Doped Perovskite and Perovskite-Related Oxides for High Temperature Redox-Active Chemical and Electrochemical Applications," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
79. C. Wolverton, "Oxygen Off-Stoichiometry and Defect Entropies in Solar Thermochemical Water Splitting Materials," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.

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80. S. Lany, “The Electronic Entropy of Charged Defect Formation and Its Impact on Thermochemical Redox Cycles,” Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
81. M. Sanders, A. Bergeson-Keller, N. Kumar, J. Pan, D. Barcellos, V. Stevanovic, S. Lany, R. O’Hayre, “The Effect of Structure on Oxygen Vacancy Formation Energy in Ce-Substituted Sr-Mn Oxides,” Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
82. S. Haile, X. Gian, “Thermochemical Trends in ABO3-Type Compounds for Solar Fuel Generation,” Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
83. O. Marina, C. Coyle, D. Edwards, J. Stevenson, “Durability Assessment of High Temperature Electrolysis Cells,” Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
84. A. Bergeson-Keller, D. Barcellos, M. Sanders, R. O’Hayre, “Study of the Reduction Thermodynamics of Sr 1-x Ce x MnO 3 Perovskites for Solar Thermochemical Hydrogen Production,” Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
85. J. Miller, I. Ermanoski, A. Ambrosini, E. Stechel, “Ammonia Synthesis in Two Cyclic Steps—Basic Thermodynamic Considerations,” Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.

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86. L. Zhu, C. Cadigan, C. Duan, J. Huang, L. Bian, L. Le, N. Sullivan, R. O'Hayre, "High-Performance Reversible Proton-Conducting Ceramic Cells for Power Generation and Energy Storage Through Ammonia," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
87. E. Stechel, I. Ermanoski, J. Miller, "Materials Thermodynamic Limits in Solar–Thermochemical Fuel Production," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.
88. I. Ermanoski, E. Stechel, J. Miller, "Thermal–Driven Oxygen Pumping in Thermochemical Fuel Production," Oral presentation at the 2019 MRS Spring Meeting and Exhibit, Phoenix, AZ, April 22–26, 2019.