

FCTO's HydroGEN AWSM Energy Materials Network Overview Webinar

Huyen N. Dinh, National Renewable Energy Laboratory

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Fuel Cell Technologies Office Webinar

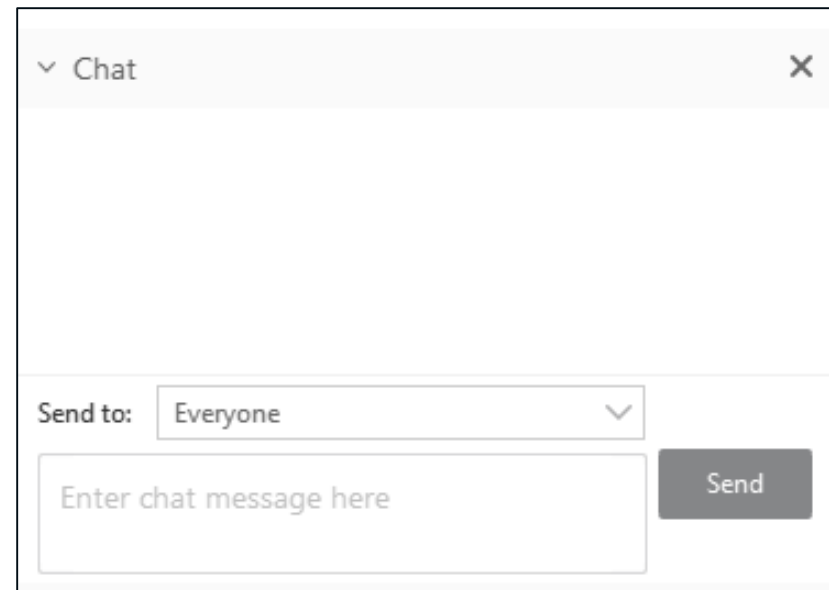
February 7, 2019



This presentation is part of the monthly webinar series provided by the U.S. Department of Energy's Fuel Cell Technologies Office (FCTO) within the Office of Energy Efficiency and Renewable Energy (EERE). Funding for research, development and innovation to accelerate progress in hydrogen and fuel cell technologies is provided by EERE FCTO.

During Q&A session:



Please type your questions to the chat box. Send to: (HOST)



The image shows a chat window titled "Chat" with a close button (X) in the top right corner. Below the title bar is a large empty text area for messages. At the bottom of the window, there is a "Send to:" dropdown menu currently set to "Everyone". Below the dropdown is a text input field with the placeholder text "Enter chat message here". To the right of the input field is a "Send" button.

Goals and Objectives of H₂ Fuel R&D at FCTO

FCTO Early-Stage R&D Areas

 Fuel Cells	 Hydrogen
<ul style="list-style-type: none">• PGM- free catalysts• Durable MEAs• Electrode performance	<ul style="list-style-type: none">• Production pathways• Delivery components• Advanced materials for storage

PGM = Platinum group metals
MEA = Membrane Electrode Assembly

H₂ Production

- Enable H₂ production at < \$2/kg utilizing diverse, domestic feedstocks

H₂ Delivery

- Reduce the cost of delivery and dispensing to \$5/kg by 2025 and ultimately \$2/kg

H₂ Storage

- Enable \$8/kWh for on-board H₂ storage cost

HydroGEN consortium supports early stage R&D in H₂ production



For more information & Engagement with HydroGEN

Go to www.h2awsm.org

For capability node lists and descriptions, technology transfer agreements and currently funded project info

When a FOA is open, first engagement should go through
h2awsm@nrel.gov

To identify and discuss capability node(s) of interest



How do I find the right resource to accelerate a solution to my materials challenge?



How do I engage with the National Labs quickly and effectively?

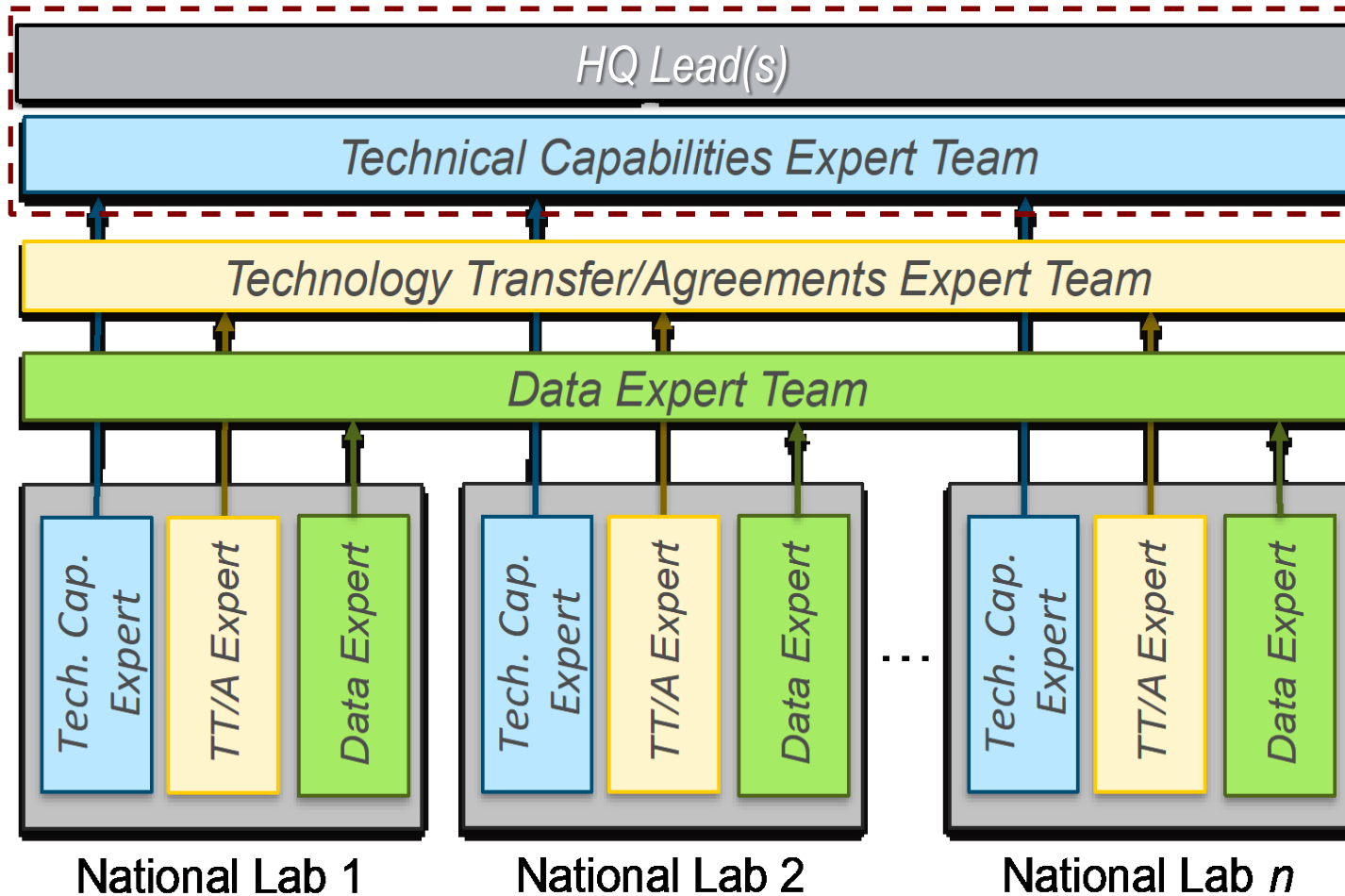
The EMN offers a common yet flexible R&D consortium model to address key materials challenges in specific high-impact clean energy technologies aimed at accelerating the tech-to-market process



- **World Class Materials Capability Network:** *Create and manage a unique, accessible set of capabilities within the DOE National Laboratory system.*
- **Clear Point of Engagement:** *Provide a single point-of-contact and concierge to direct interested users (e.g. industry research teams) to the appropriate laboratory capabilities, and to facilitate efficient access.*
- **Data and Tool Collaboration Framework:** *Capture data, tools, and expertise developed at each node such that they can be shared and leveraged throughout the EMN and in future programs. Establish data repositories and, where appropriate, distribute data to the scientific community and public. Accelerate learning and development through data analysis using advanced informatics tools.*
- **Streamlined Access:** *Facilitate rapid completion of agreements for external partners, and aggressively pursue approaches to reduce non-technical burden on organizations seeking to leverage the EMN for accelerated materials development.*



Consortium Steering Teams



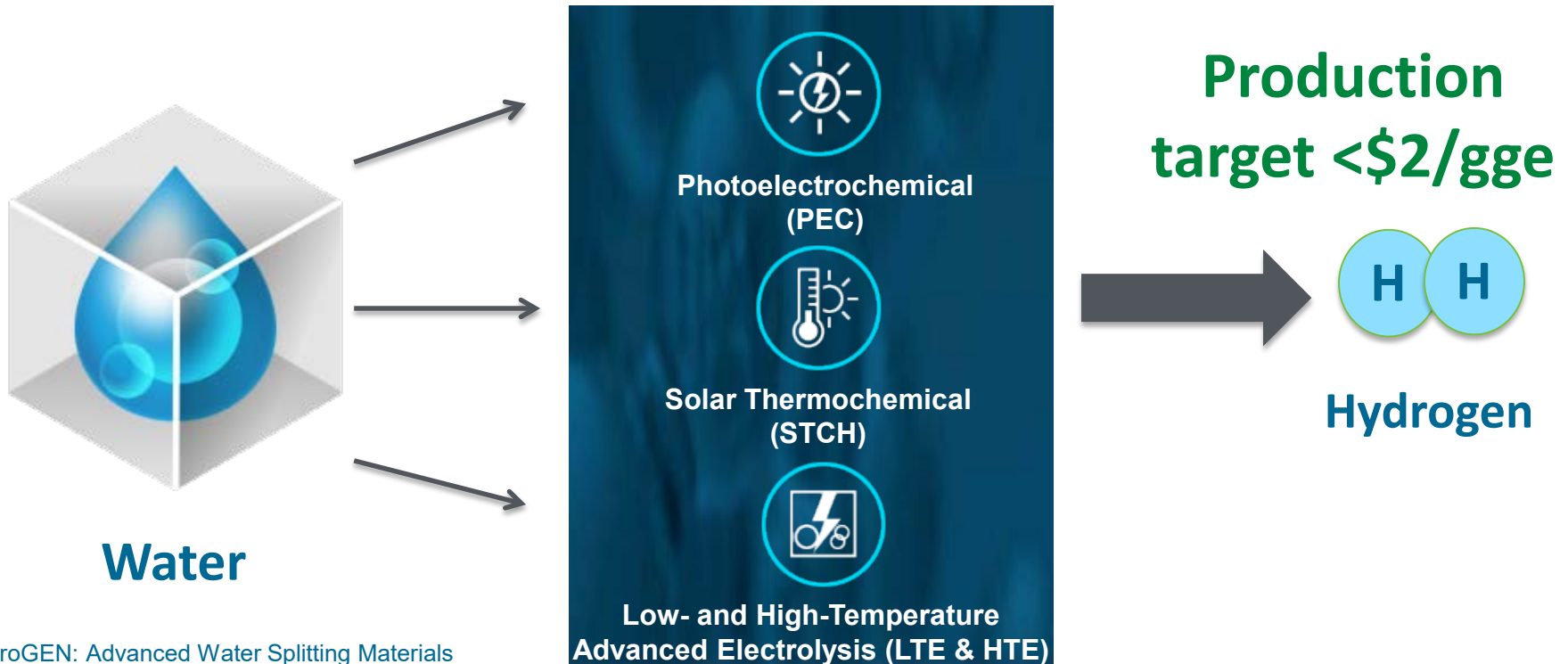


Advanced Water-Splitting Materials (AWSM)

**AWSM Consortium
Six Core Labs:**



Accelerating R&D of innovative materials critical to advanced water splitting technologies for clean, sustainable, and low cost H₂ production, including:





HydroGEN Steering Committee



Huyen Dinh
(Director)



Adam Weber
(Deputy Director)



Anthony McDaniel
(Deputy Director)



Richard Boardman



Tadashi Ogitsu



Donald Anton



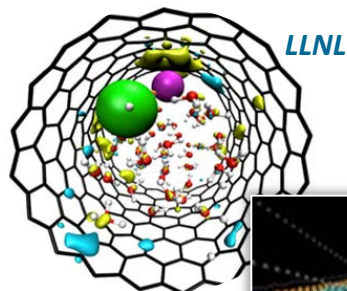
Eric Miller and Katie Randolph, DOE-EERE-FCTO



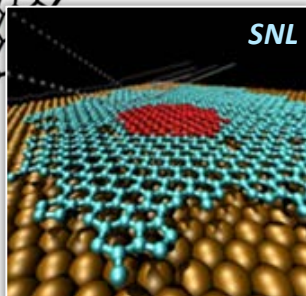
HydroGEN-AWSM Consortium

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

Materials Theory/Computation

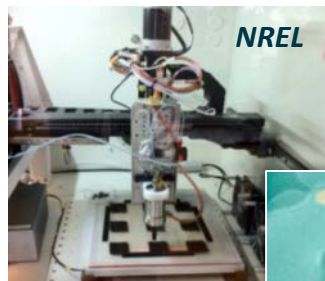


Bulk & interfacial models of aqueous electrolytes

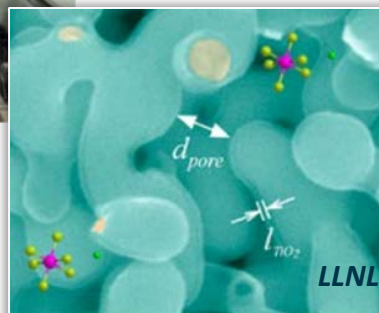


LAMMPS classic molecular dynamics modeling relevant to H_2O splitting

Advanced Materials Synthesis



High-throughput spray system for electrode fabrication

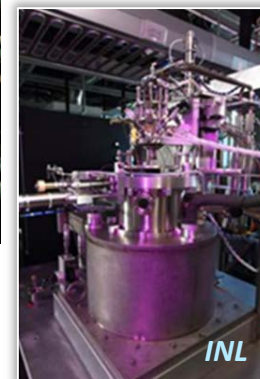


Conformal ultrathin TiO_2 ALD coating on bulk nanoporous gold

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



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

Search

[Reset filtering](#)

CAPABILITY CLASS

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

WATER-SPLITTING TECHNOLOGY

- High-Temperature Electrolysis
 - HTE 1 HTE 2 HTE 3
- Low-Temperature Electrolysis
 - LTE 1 LTE 2 LTE 3
- Photoelectrochemical
 - PEC 1 PEC 2 PEC 3
- Solar Thermochemical
 - STCH 1 STCH 2
 - STCH 3
- Hybrid Thermochemical
 - HT 1 HT 2 HT 3

Node Readiness Categories

NATIONAL LABORATORY

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

Showing 1 to 12 of 82 entries

1 2 3 4 Next

Show 12

Ab Initio Modeling of Electrochemical Interfaces


LLNL PEC 1, LTE 2

Advanced Electron Microscopy

SNL HTE 1, LTE 1, PEC 1, STCH 1

Advanced Materials for Water Electrolysis at Elevated Temperatures

INL HTE 2





HydroGEN FOA-Awarded Projects

21 proposals selected, negotiated, and awarded
44 unique capabilities being utilized across six core labs

Advanced Electrolysis (10)

LTE (5)

HTE (5)

PEC (5)

**Benchmarking &
Protocols (1)**

STCH (5)

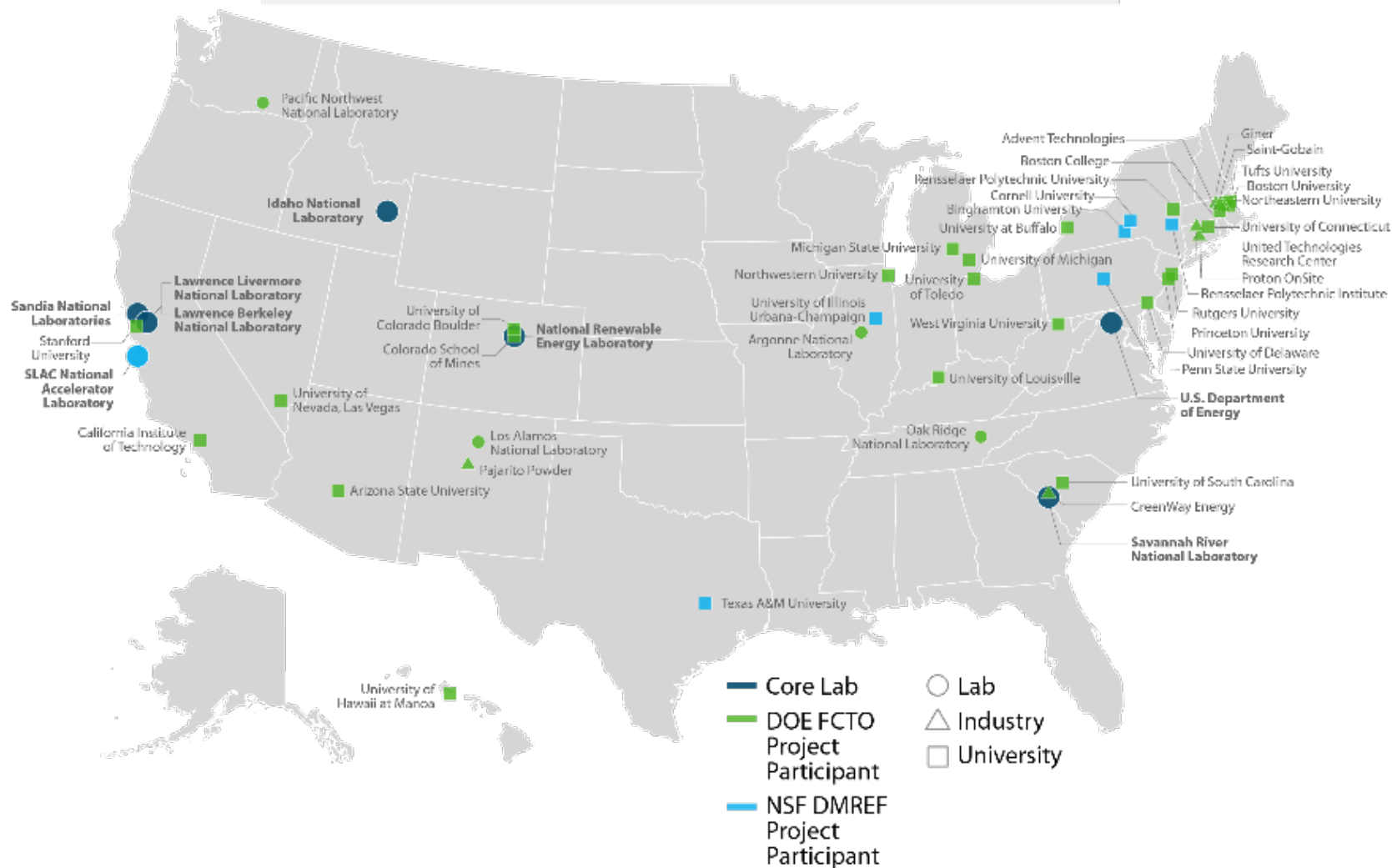
2-Step MO_x (4)
Hybrid cycle (1)





National Innovation Ecosystem

11 Labs 7 Companies 30 Universities 2 Funding Agencies



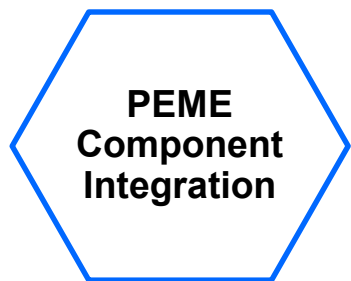
HydroGEN is vastly collaborative and focused on early-stage R&D



A Balanced AWSM R&D Portfolio



Low Temperature Electrolysis (LTE) (5 Projects)



PEM Electrolysis

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

AEM Electrolysis

High Temperature Electrolysis (HTE) (5 Projects)

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

O²⁻ conducting SOEC

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

H⁺ conducting SOEC

Photoelectrochemical (PEC) (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) (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



Low Temperature Electrolysis (45 Nodes)

Low Temperature Electrolysis (LTE)

- Proton Exchange Membrane (PEM)
- Alkaline Exchange Membrane (AEM)

13 nodes used by current LTE projects

LTE Node Labs



Support through:

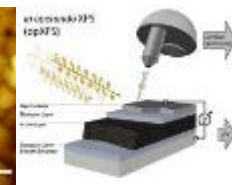
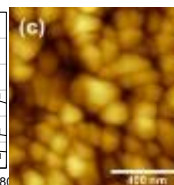
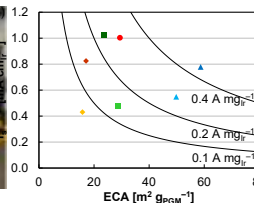
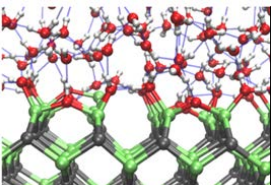


Personnel
Equipment
Expertise
Capability
Materials
Data

LTE Projects



Northeastern University
Center for Renewable Energy Technology





High Temperature Electrolysis (39 Nodes)

High Temperature Electrolysis (HTE)

- Oxygen Conducting SOEC (o-SOEC)
- Proton Conducting SOEC (p-SOEC)

6 nodes used by current HTE projects

HTE Node Labs



Support through:



Personnel
Equipment
Expertise
Capability
Materials
Data

HTE Projects



United Technologies Research Center

UCONN

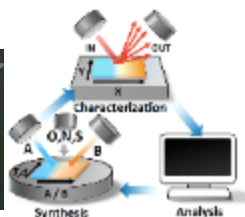
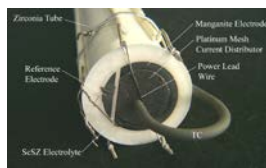
Northwestern



West Virginia University



SAINT-GOBAIN RESEARCH NORTH AMERICA





Photoelectrochemical Water Splitting (56 Nodes)

PEC: Photoelectrochemical (PEC) Water Splitting

17 nodes used by current PEC projects

PEC Node Labs

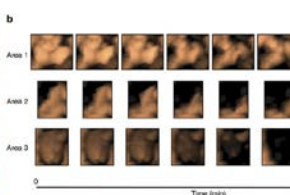
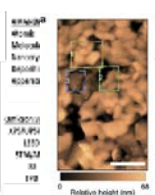
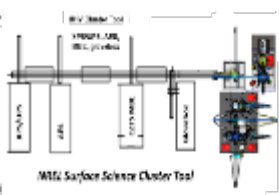
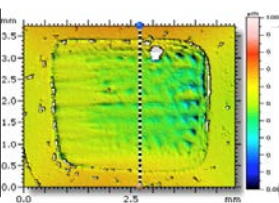
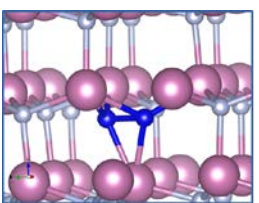


Support through:



Personnel
Equipment
Expertise
Capability
Materials
Data

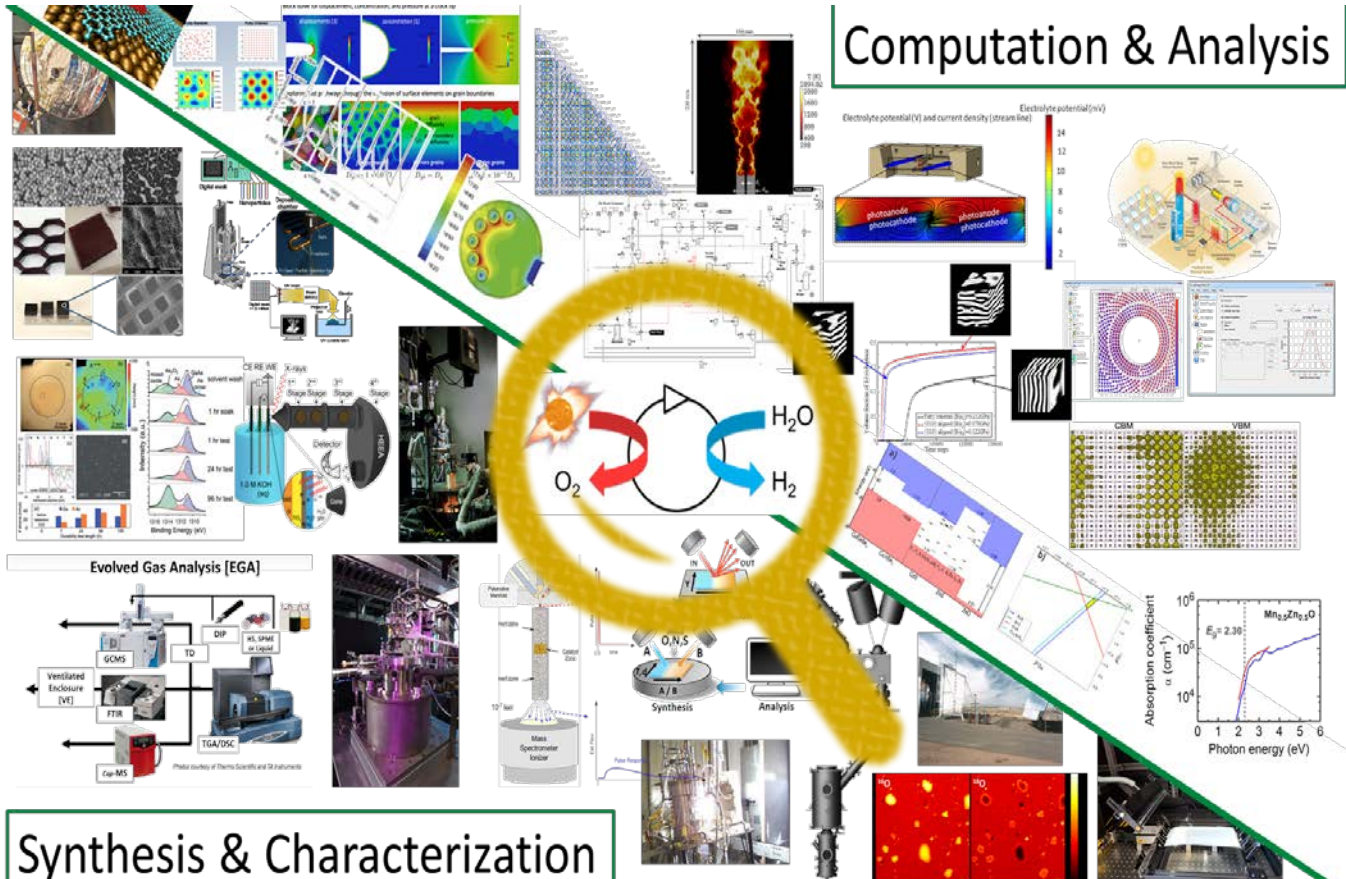
PEC Projects





Solar and Hybrid Thermochemical (39 Nodes)

Computation & Analysis



Synthesis & Characterization

11 nodes from 5 National Labs supporting 5 STCH projects

STCH Projects

ASU
Arizona State University

Northwestern

Greenway Energy LLC
Engineering consultant in Aiken County, South Carolina

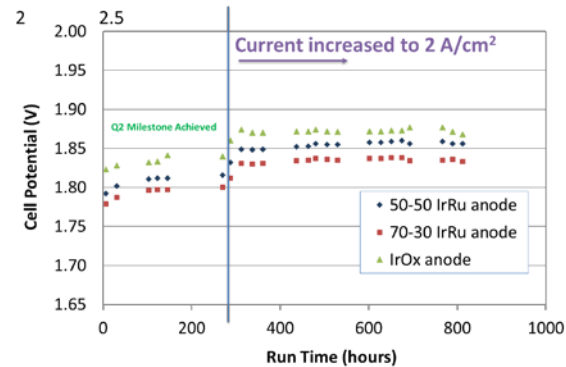
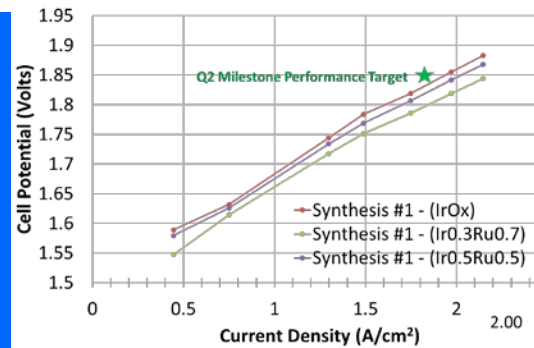




HydroGEN Collaborative R&D Technical Highlights

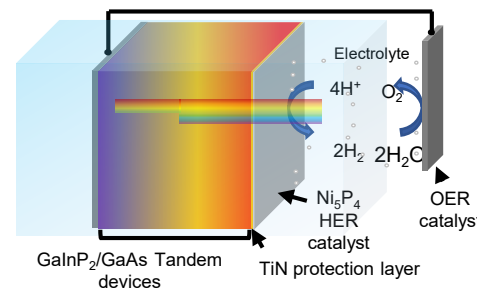
Low Temperature Electrolysis (LTE)

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 H₂, a significant improvement over the state-of-the-art cell efficiency of 53 kWh/kg.

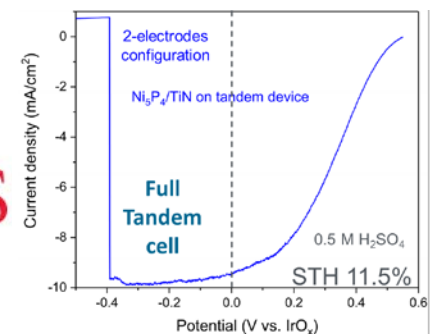


Photoelectrochemical (PEC) Water Splitting

NREL's high performance photoabsorber (GaInP₂/GaAs), integrated with Rutgers' PGM-free electrocatalysts (LiCoO₂ and Ni₅P₄) 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





HydroGEN Collaborative R&D Technical Highlights

High Temperature Electrolysis (HTE)

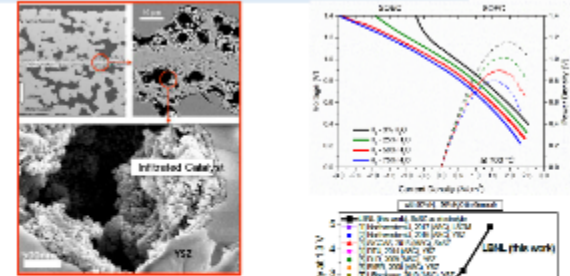
Using Northwestern University catalyst, YSZ electrolyte ($(\text{ZrO}_2)_{0.92}(\text{Y}_2\text{O}_3)_{0.08}$), and LBNL Metal-Supported Solid Oxide Cell and INL Advanced HTE testing nodes, the collaboration **demonstrated a metal-supported SOEC for the first time in electrolysis mode, with the highest performance for oxygen-conducting type electrolysis cells to-date and promising stability.**

Solar Thermochemical (STCH) Water Splitting

The University of Colorado Boulder, with NREL's DFT node, was able to develop and apply 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 are 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.**

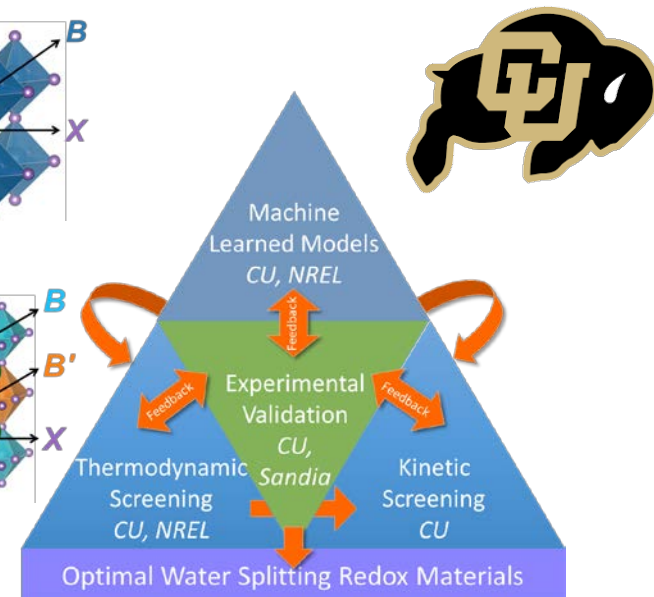
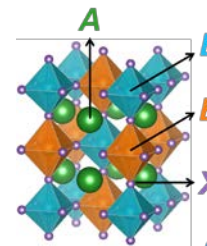
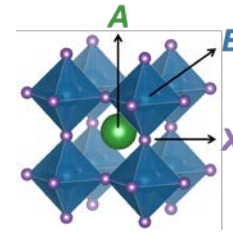
Northwestern

Symmetric Structure Metal-Supported Solid Oxide Electrolysis Cells (MS-SOECs)



- Advantages include low cost, high strength, thermal cycling capability
- First MS-SOEC results
- Initial performance excellent
- Fast degradation

HydroGEN: Advanced Water Splitting Materials

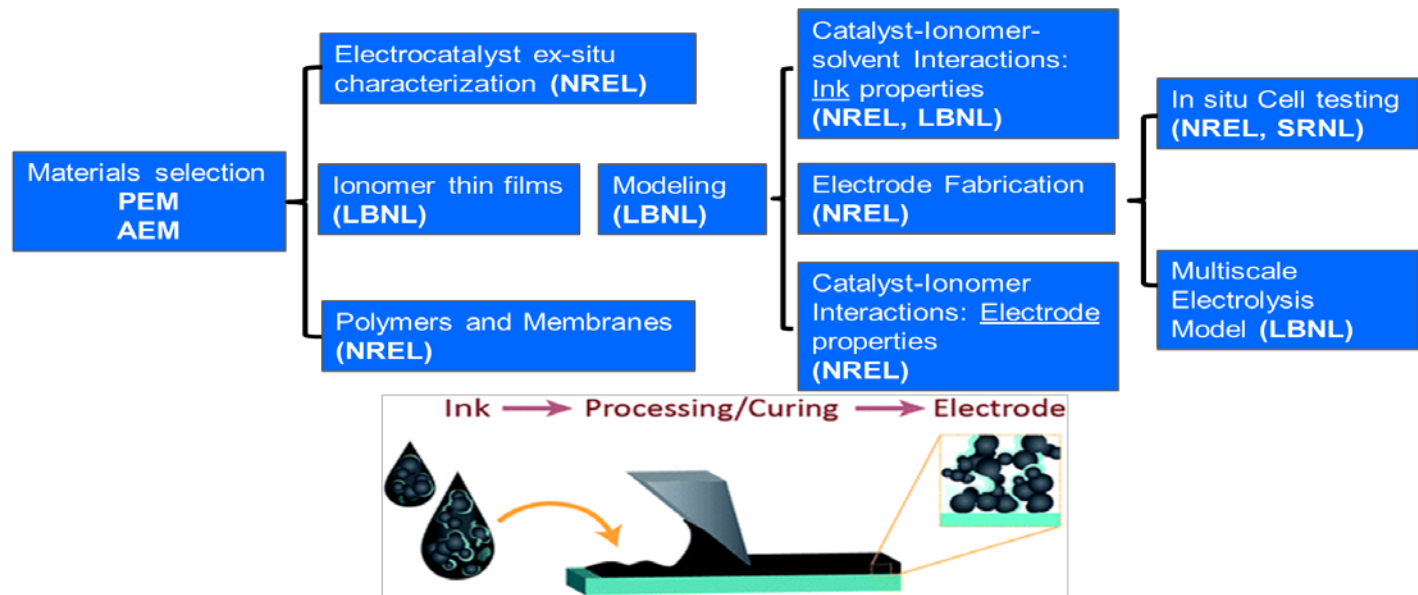




Five New Collaborative “Supernodes” Developed to Accelerate AWSM R&D



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



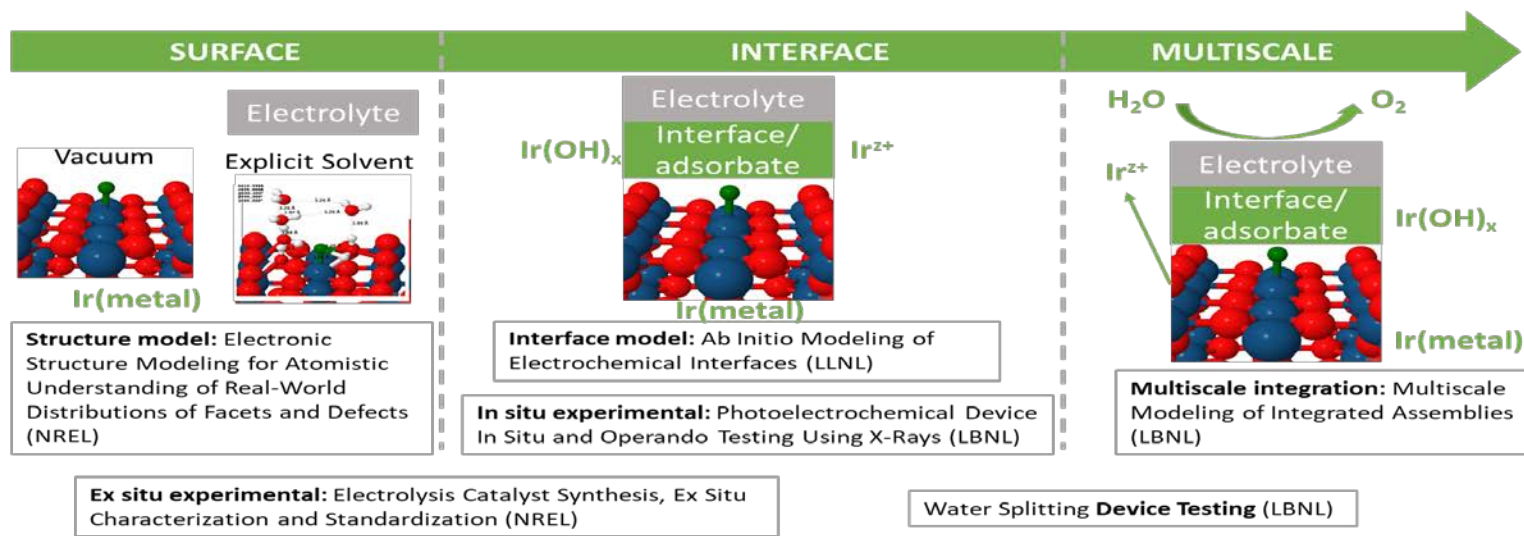
Outcome: Better integration between ex-situ and in-situ performance, more relevant ex-situ testing, and improved material specific component development to achieve optimized electrolyzer cell performance and durability.



Five New Collaborative “Supernodes” Developed to Accelerate AWSM R&D



2. OER Supernode : Understanding OER Across pH Ranges Through Multiscale, Multi-Theory Modeling (LBNL, LLNL, NREL; 6 Nodes)



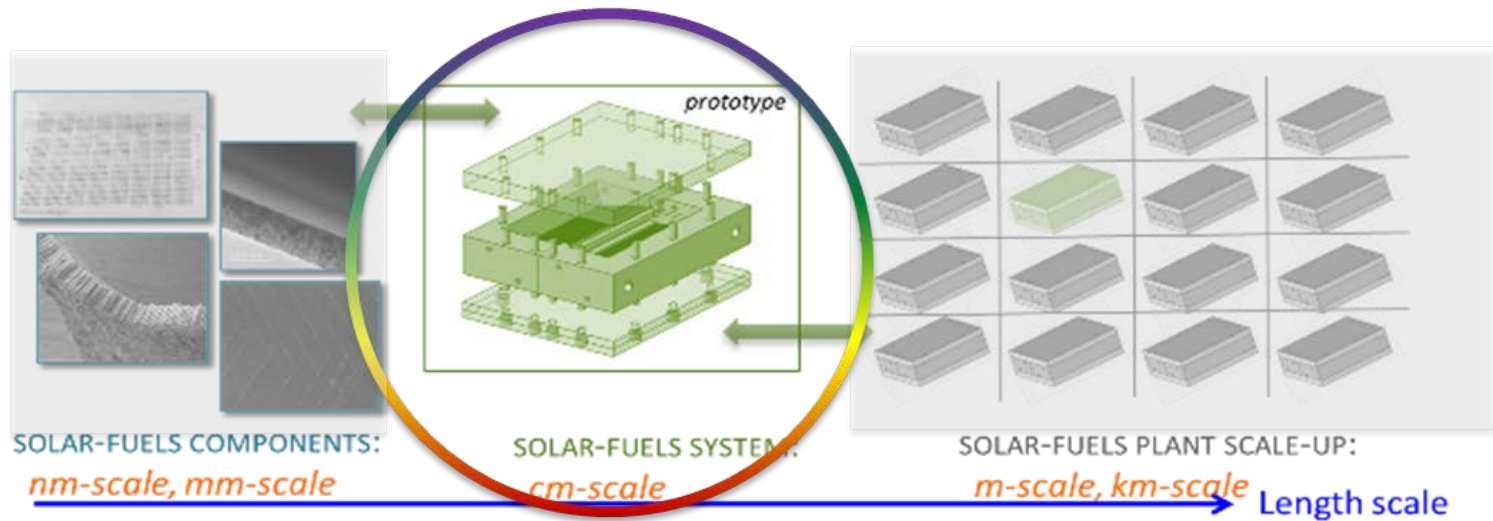
Outcome: Address knowledge gaps about OER and demonstrate a multiscale multi-theory methodology.



Five New Collaborative “Supernodes” Developed to Accelerate AWSM R&D



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



Outcome: *Understand integration issues and emergent degradation mechanisms of PEC devices at relevant scale, and demonstrate an integrated and durable 50 cm² PEC panel.*



Five New Collaborative “Supernodes” Developed to Accelerate AWSM R&D



4. HTE Supernode : Supernode Capability to Characterize HTE Electrode Microstructure Evolution (INL, NREL, LBNL, LLNL; 6 Nodes)

Processing ↔ Structure ↔ Properties ↔ Performance

Cell Fabrication

Analysis

Measurements

Catalyst Infiltration

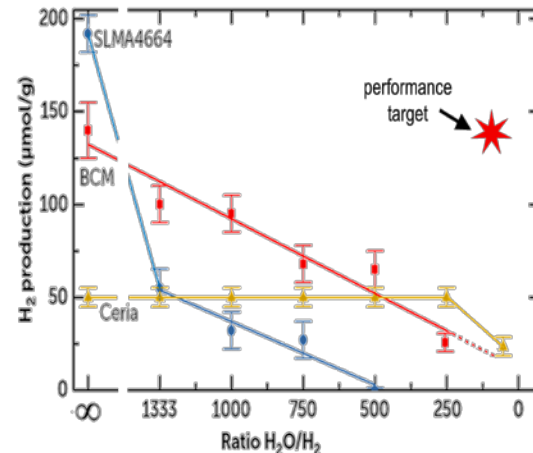
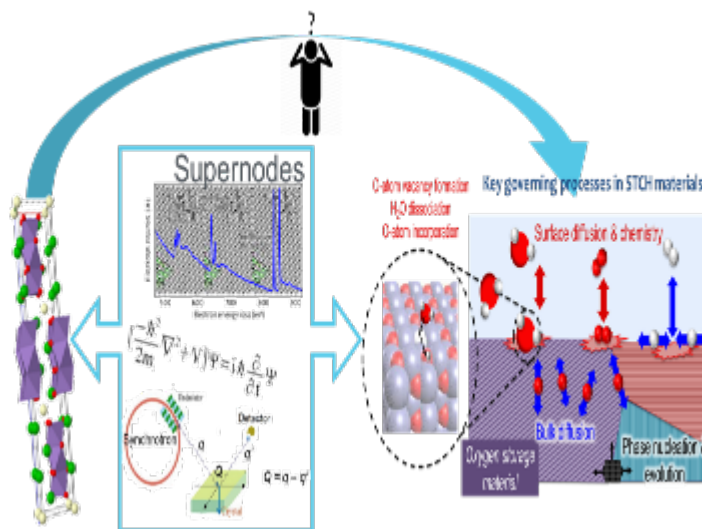
Outcome: A deeper understanding of HTE electrode microstructure evolution as a function of local solid-oxide composition and operating conditions to develop more active, longer-life electrodes.



Five New Collaborative “Supernodes” Developed to Accelerate AWSM R&D



5. STCH Supernode : Develop Atomistic Understanding of the Layered Perovskite $Ba_4CeMn_3O_{12}$ (BCM) and its Polytypes (SNL, NREL, LLNL; 7 Nodes)



Outcome: A comprehensive understanding of Mn’s local structure in BCM will lead to novel pathways for modifying and improving STCH perovskites.



4 New NSF DMREF / DOE EERE HydroGEN EMN Projects

NSF DMREF PSU LTE



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



High Temperature Defects: Linking Solar Thermochemical 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



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



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

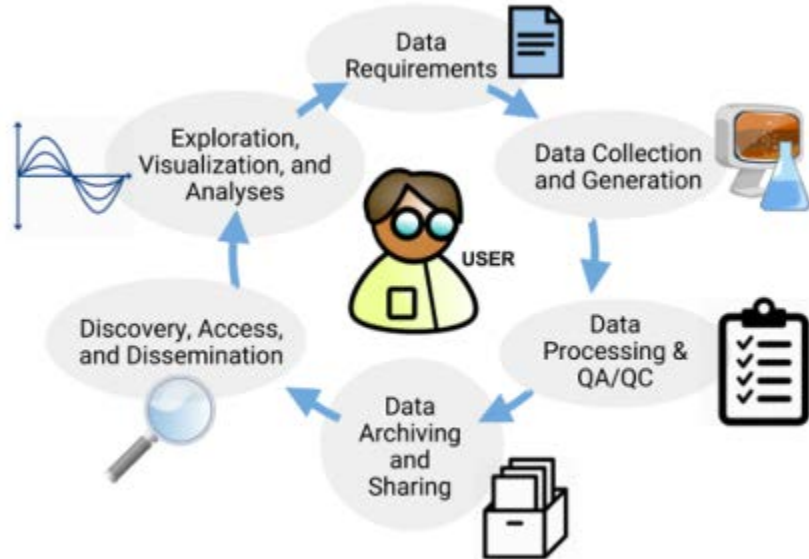
- Jinghua Guo
- David Prendergast



HydroGEN Data Hub: Making digital data accessible

A Researcher Centric Approach

The HydroGEN Data Hub currently has
>170 users, >4050 files



<https://datahub.h2awsm.org/>



Data Hub implemented in May 2017

- Secure project space for team members
- View and download project data
- Metadata tools to support advanced search
- Data plug-ins for visualization and graphing of data





Technology Transfer Agreements (TT/A)

Non-Disclosure Agreement (NDA)

Information Disclosure

Intellectual Property Management Plan (IPMP)

IP Protection

➤ Streamlined Access

Materials Transfer Agreement (MTA)

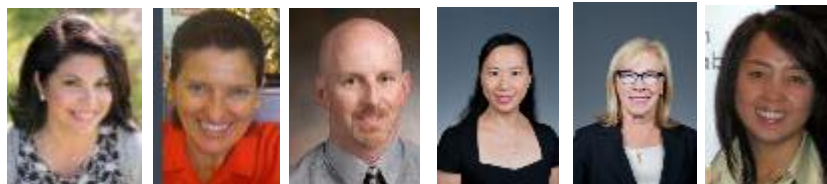
Freedom to Operate

Cooperative Research and Development Agreement (CRADA)

Collaboration

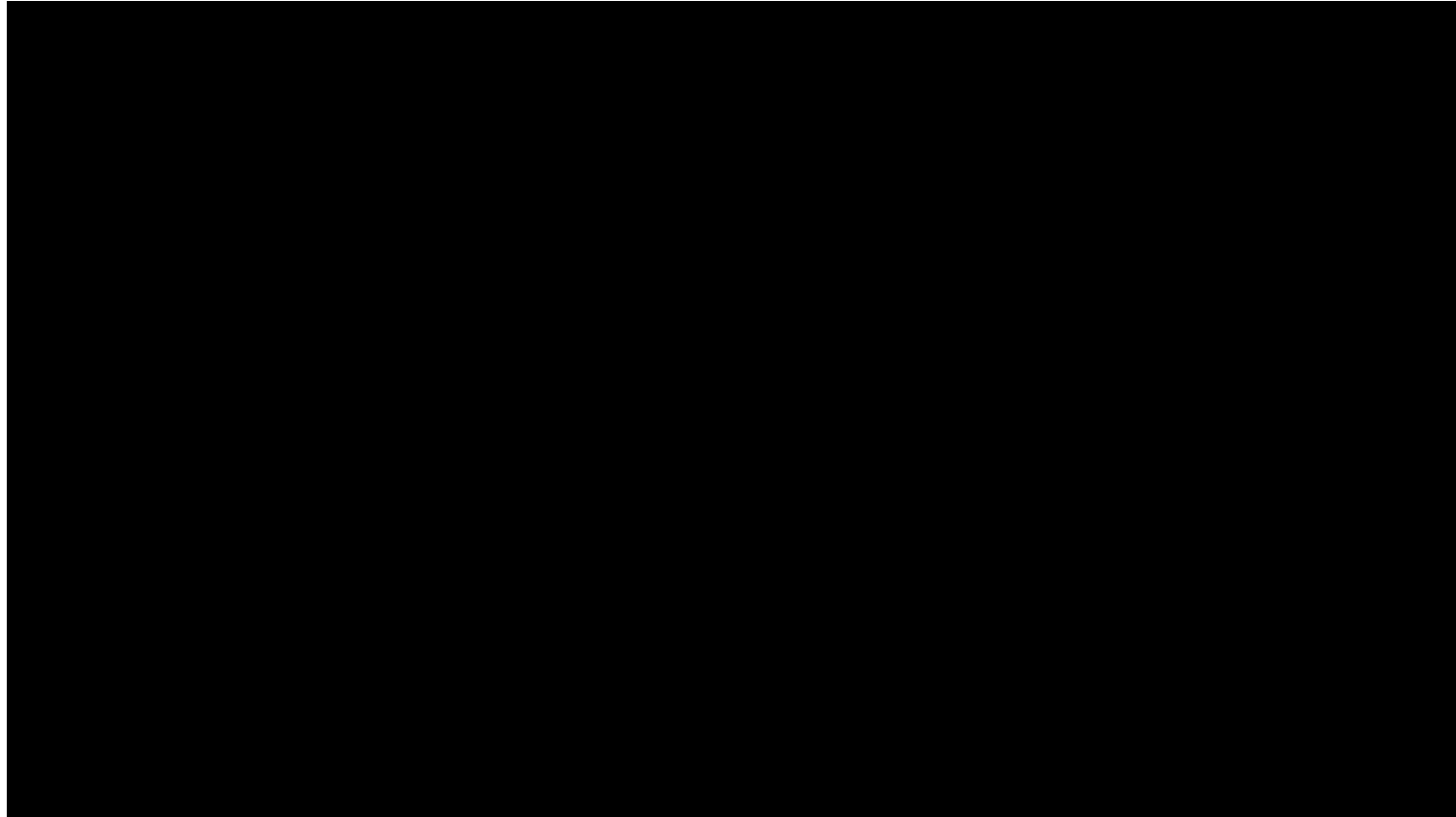
- ✓ Four standard, pre-approved TT/A between all consortium partners
- ✓ Executed all 21 project NDAs and 2 MTAs

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





Working with HydroGEN: Testimonials



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.



Useful HydroGEN-Related Links

- 2016 HydroGEN Webinars (good capability descriptions)
 - [HydroGEN Consortium Overview, Part 1 of 3: Photoelectrochemical \(PEC\) Water Splitting](#)
 - [HydroGEN Consortium Overview, Part 2 of 3: Electrolysis](#)
 - [HydroGEN Consortium Overview, Part 3 of 3: Solar Thermochemical \(STCH\) Hydrogen Production](#)
- [2017 HydroGEN-FOA Awarded Project Kick-Off Presentations](#)
- [2018 HydroGEN EMN AMR Presentations and Posters](#)
- [HydroGEN Website](#)
 - [Technology Transfer Agreement Types](#)
 - [Video testimonial](#)
- [HydroGEN Data Hub](#)
- [DOE EERE Energy Materials Networks](#)

Acknowledgements



Energy Materials Network
U.S. Department of Energy



HydroGEN
Advanced Water Splitting Materials

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Katie Randolph



David Peterson



James Vickers



Eric Miller





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Go to www.h2awsm.org

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h2awsm@nrel.gov

To identify and discuss capability node(s) of interest

Acknowledgements



Energy Materials Network
U.S. Department of Energy



HydroGEN
Advanced Water Splitting Materials

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Adam Weber

LTE Project Leads

Kathy Ayers
Chris Capuano
Hoon Chung
Yu Seung Kim
Di-Jia Liu
Sanjeev Mukerjee

Research Teams



University at Buffalo
The State University of New York



Rensselaer



**PAJARITO
POWDER**
PURE CELL CATALYSIS



Advent



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



Northeastern University
Center for Renewable Energy Technology



School of
Engineering



Acknowledgements



Energy Materials Network
U.S. Department of Energy



HydroGEN
Advanced Water Splitting Materials

Node Experts

Dong Ding
Michael Tucker
Zhiwen Ma
James O'Brien
Carl Stoots
Andriy Zakutayev

HTE Project Leads

Scott Barnett
Tianli Zhu
Prabhakar Singh
Xingbo Liu
John Pietras

Research Teams



**United Technologies
Research Center**

UConn



West Virginia University

Northwestern

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SAINT-GOBAIN RESEARCH NORTH AMERICA



Pacific Northwest
NATIONAL LABORATORY

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Acknowledgements



Energy Materials Network
U.S. Department of Energy



HydroGEN
Advanced Water Splitting Materials

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Save the Date and Sign up for Our Newsletter

**All relevant DOE offices and other federal agencies
working on hydrogen and fuel cell technologies at
Annual Merit Review (AMR)**

2019 AMR – April 29 – May 1
Crystal City, VA
www.hydrogen.energy.gov

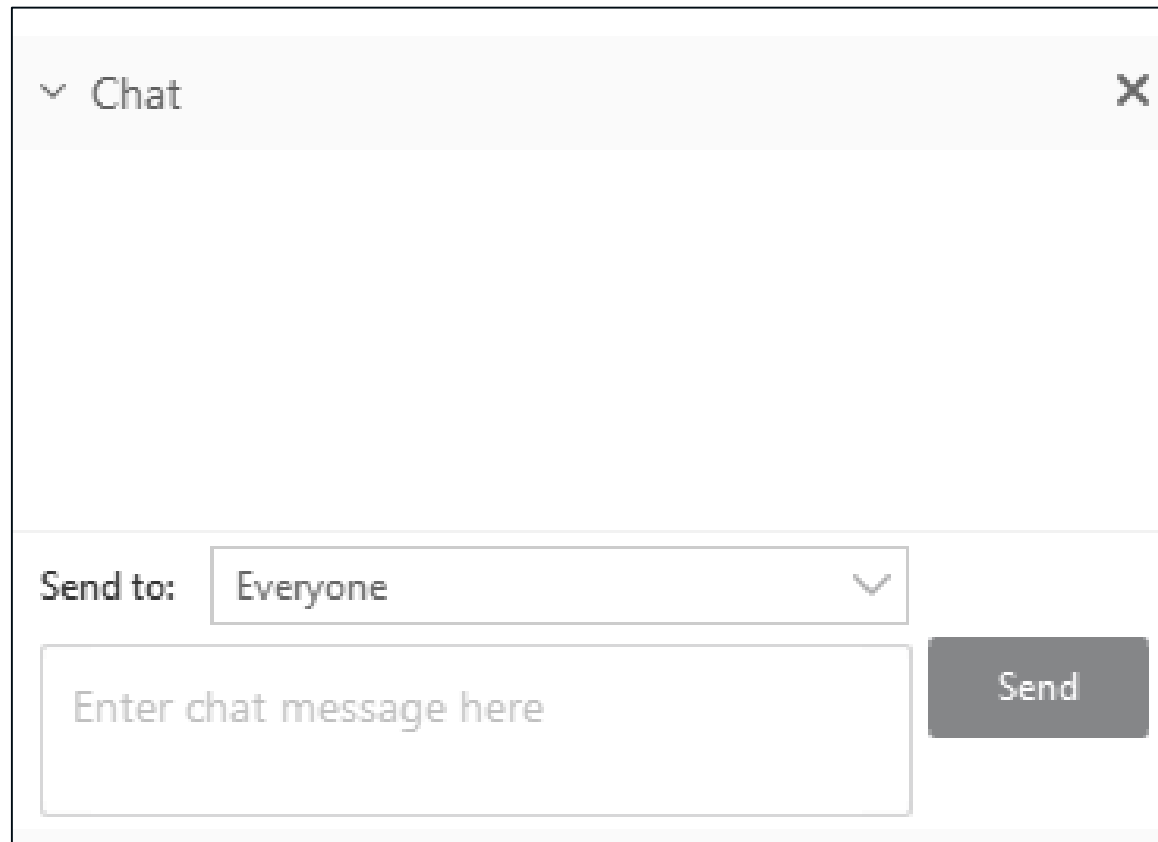
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Backup Slides



HydroGEN Capability Nodes

Node evaluation criteria:

1. **Relevant** to HydroGEN water splitting pathways
 2. **Available** resources and associated expert(s) to support the capability and available to external stakeholders
 3. **Unique** to the national laboratory system; comprise expertise, tools, and techniques
- **Other Considerations:**
 - **Node readiness category**

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

- Nodes comprise tool, technique, and expertise including uniqueness
- Category refers to availability, readiness and relevance to AE and not necessarily the expense and time commitment

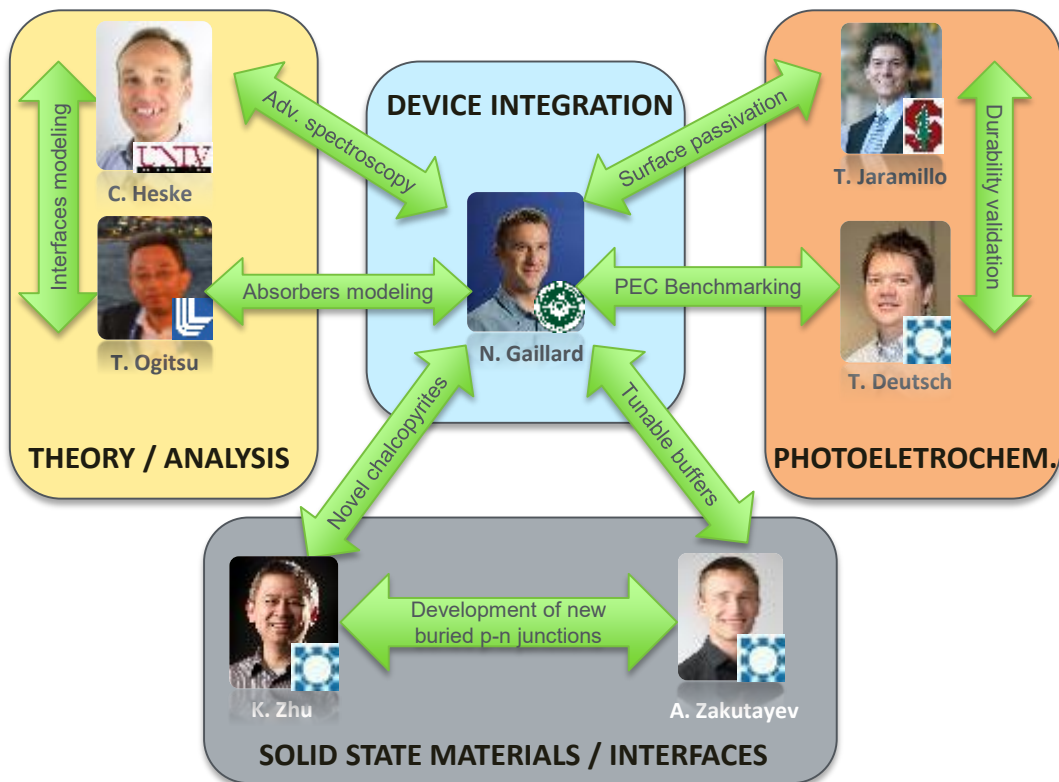
Capability nodes are regularly updated and new ones are added



Collaboration Example: U Hawaii/HydroGEN Node Interactions

Academia-EMN Node interaction

Integrated Theory, Analysis, Synthesis and Testing



Computational Materials Diagnostics and Optimization Node (T. Ogitsu).

- ▶ **Role:** theoretical modeling of novel materials.
- ▶ **Benefit to this program:** defines synthesis conditions and thermodynamic stability of chalcopyrite candidates.

I-III-VI Compound Semiconductors for Water-Splitting Node (K. Zhu)

- ▶ **Role:** synthesis of high-purity material systems.
- ▶ **Benefit to this program:** "ideal" vacuum-based chalcopyrites used to test alloying/doping strategies.

High-Throughput Thin Film Combinatorial Capabilities Node (A. Zakutayev)

- ▶ **Role:** develop n-type buffers with tunable 'energetics'
- ▶ **Benefit to this program:** accelerates material discovery for improved interfaces.

Corrosion Analysis of Materials Node (T. Deutsch)

- ▶ **Role:** supports development of surface passivation against photo-corrosion.
- ▶ **Benefit to this program:** provide access to unique instrumentation to identify corrosion mechanisms.



HydroGEN Benchmarking: Advanced Water Splitting Technologies Project

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:

- 4 AWSM Questionnaires
- 4 AWSM Test Frameworks
- 2 Benchmarking Newsletters
- 2 Working Group Meetings
- 3 Conference Presentations
- > 80 Capability Nodes Assessed



- *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***