



Energy Materials Network
U.S. Department of Energy



HydroGEN
Advanced Water Splitting Materials

An EMN Model for Early R&D

H.N. Dinh, K. Randolph, E. Miller

Presenter: Huyen Dinh, NREL

Date: 2/14/2018

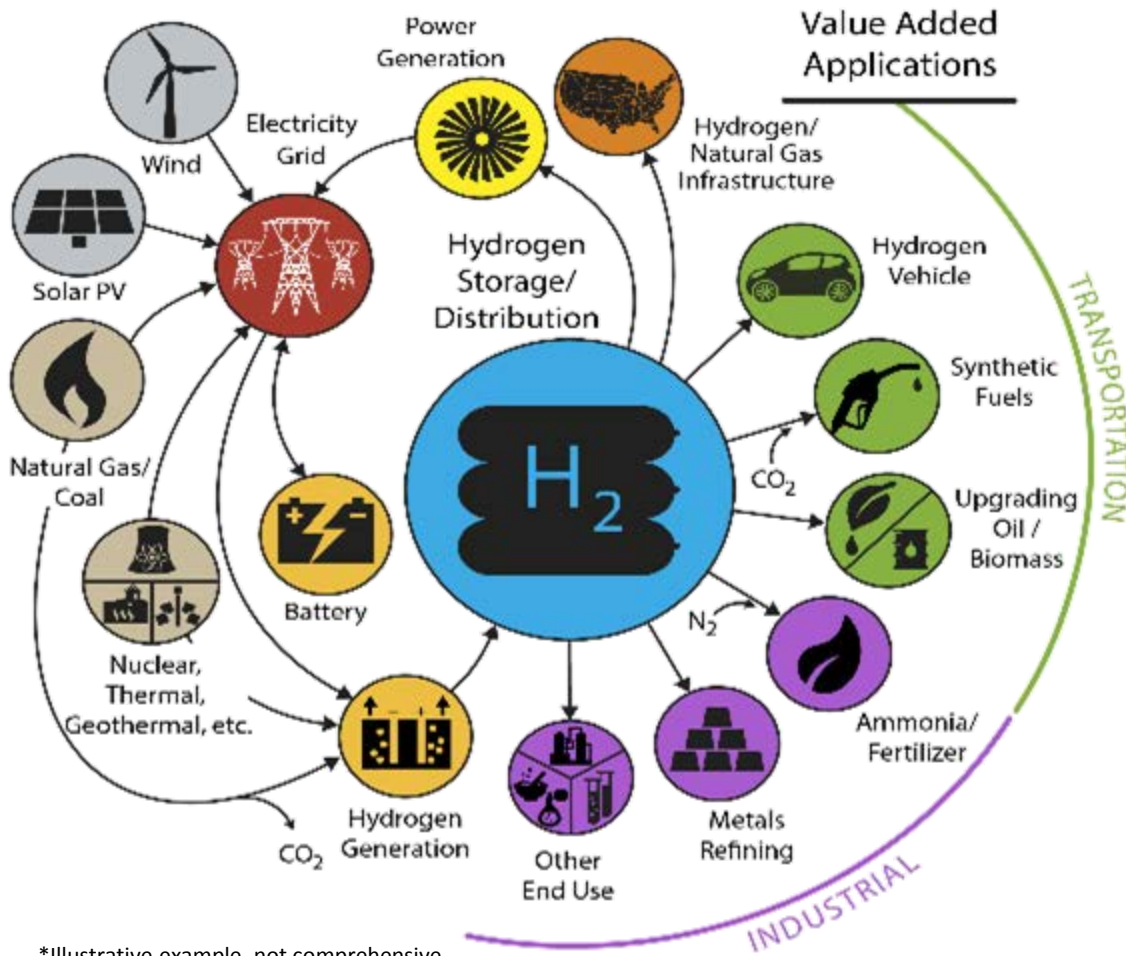
**Venue: 2018 DOE Hydrogen and Fuel Cell
Technical Advisory Committee**

This presentation does not contain any proprietary, confidential, or otherwise restricted information.



H2@Scale Energy System Vision

Transportation & Beyond



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

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

*Illustrative example, not comprehensive
Adapted from NREL, Lab Big Idea Team

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

Energy Materials Network (EMN)

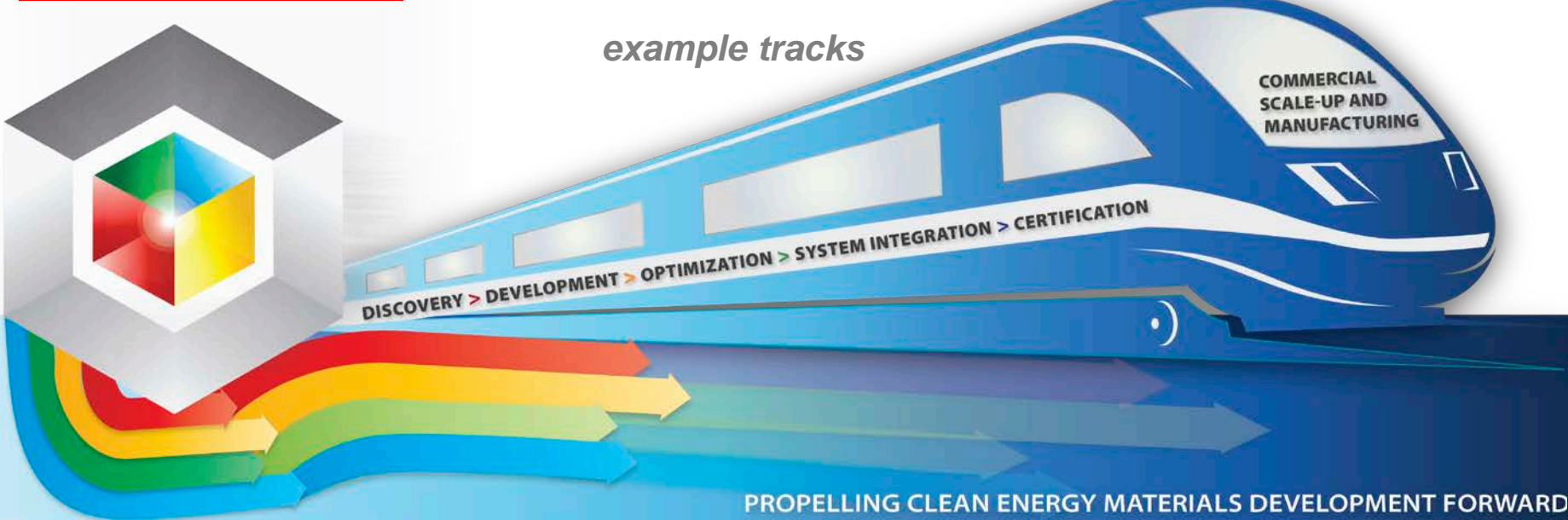
DOE's EMN aims to accelerate early-stage applied R&D in materials tracks aligned with some of the nation's most pressing sustainable energy challenges

Lightweight Materials for Vehicles

Durable Materials for Solar Modules

Advanced Water Splitting Materials for Hydrogen Production

Next-Generation Electro-catalysts for Fuel Cells



Accelerating early-stage materials R&D for energy applications

Bridging Science and Application

industry pull



product development framed by end-use process & manufacturing requirements

manufacturing

deployment

qualification

*systems
integration*

optimization

*design &
component
development*

discovery

EMN resource network facilitating materials innovations



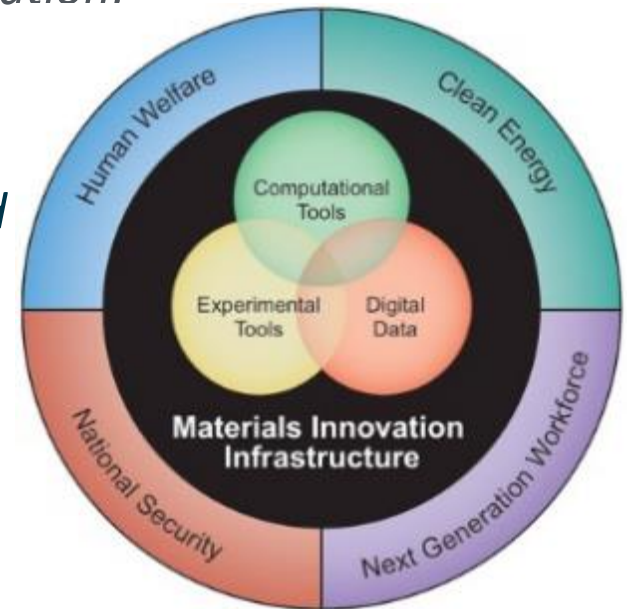
scientific push

- Lab-led EMN Consortia rely on *industry pull* and *scientific push* to work together to accelerate R&D of important clean energy technologies

Harnessing the Power of the Latest Materials R&D Methods

Foundation in Modern Materials R&D

- 1) **Leading a culture shift in materials research** *to encourage and facilitate an integrated team approach that links computation, data, and experiment and crosses boundaries from academia to industry;*
- 2) **Integrating experiment, computation, and theory** *and equipping the materials community with the advanced tools and techniques to work across materials classes from research to industrial application:*
- 3) **Making digital data accessible** *including combining data from experiment and computation into a searchable materials data infrastructure and encouraging researchers to make their data available to others;*
- 4) **Creating a world-class materials workforce** *that is trained for careers in academia or industry, including high-tech manufacturing jobs.*



Ground-breaking energy materials research is vital to U.S. interests

National Laboratory-Led Consortia



Energy Materials Network

U.S. Department of Energy

***World Class Research Resources & Expertise
in the Department's National Laboratories***

Predictive
Simulation
Across Scales

Synthesis &
Characterization

High-throughput
Screening

End Use
Performance

Process
Scalability

Process
Control

Real-time
Characterization

Reliability
Validation

Data Management & Informatics

***Organized in Consortia Focused on Specific
Key Energy Challenges***

Seven EMN consortia have been successfully deployed to date





Core Labs

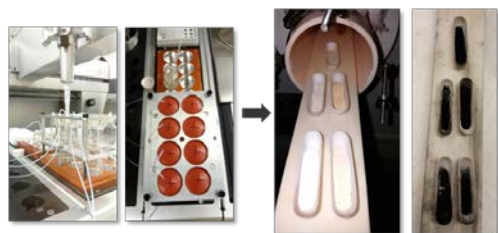


Accelerating the discovery & development of innovative catalyst and electrode materials critical to advanced platinum group metal-free fuel cell technologies

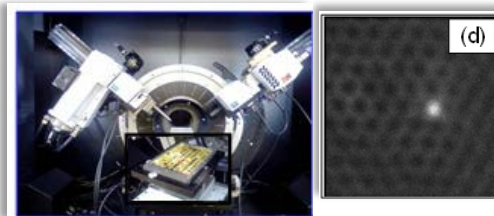
➤ *Comprising 27 world-class capabilities and expertise in:*

- Catalyst synthesis, characterization, processing, & manufacturing
- High-throughput, combinatorial techniques
- Advanced computational tools

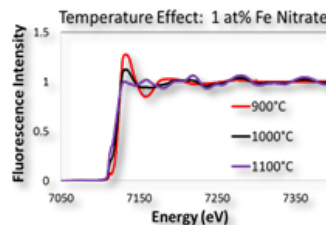
Synthesis, Processing and Manufacturing



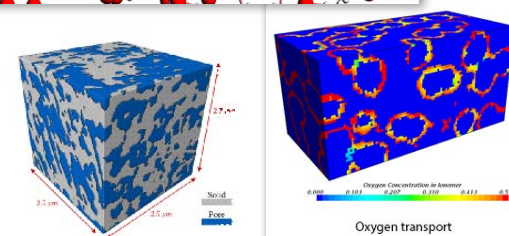
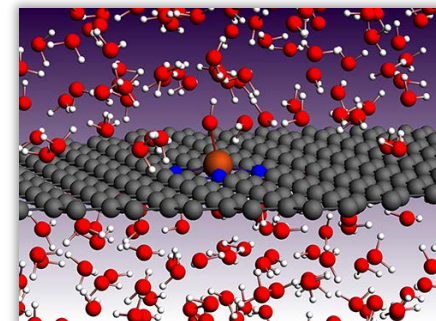
Characterization and Synthesis



Fe K-Edge EXAFS



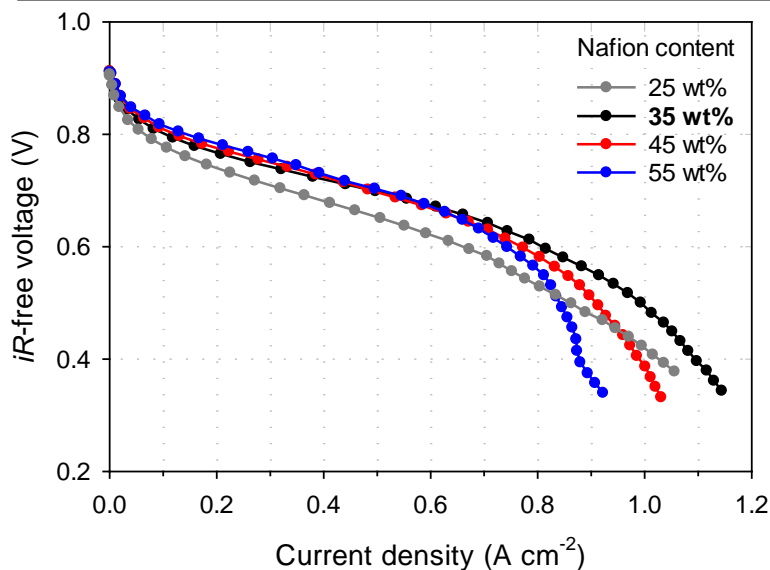
Computation, Modeling & Data Management



Performance Improvement

- Improved PGM-free H₂-air as-measured performance **by 40%** versus 2016 status and by 22 mA cm⁻² versus 2017 AMR status by using Zn as a pore-forming component in the (CM+PANI)-Fe-C catalyst synthesis and optimizing electrode ionomer content.

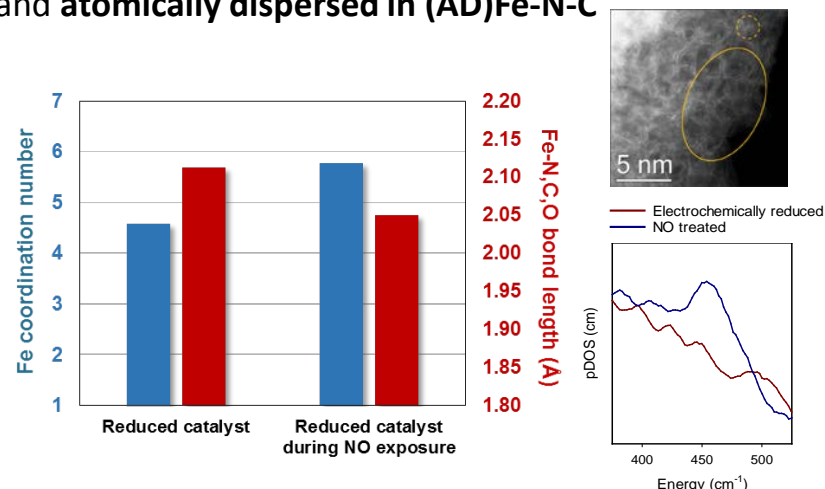
Anode: 0.3 mg_{Pt} cm⁻² Pt/C H₂, 200 sccm, 1.0 bar H₂ partial pressure; Cathode: ca. 4.8 mg cm⁻² catalyst loading, air, 200 sccm, 1.0 bar air partial pressure; Membrane: Nafion®, 211; Cell: 5 cm², 80 °C



- Increased ORR activity for atomically-dispersed Fe-N-C catalyst **by 20 mV** at $E_{1/2}$

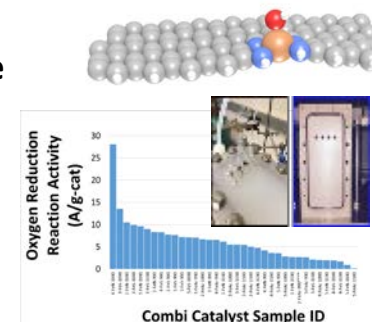
Characterization

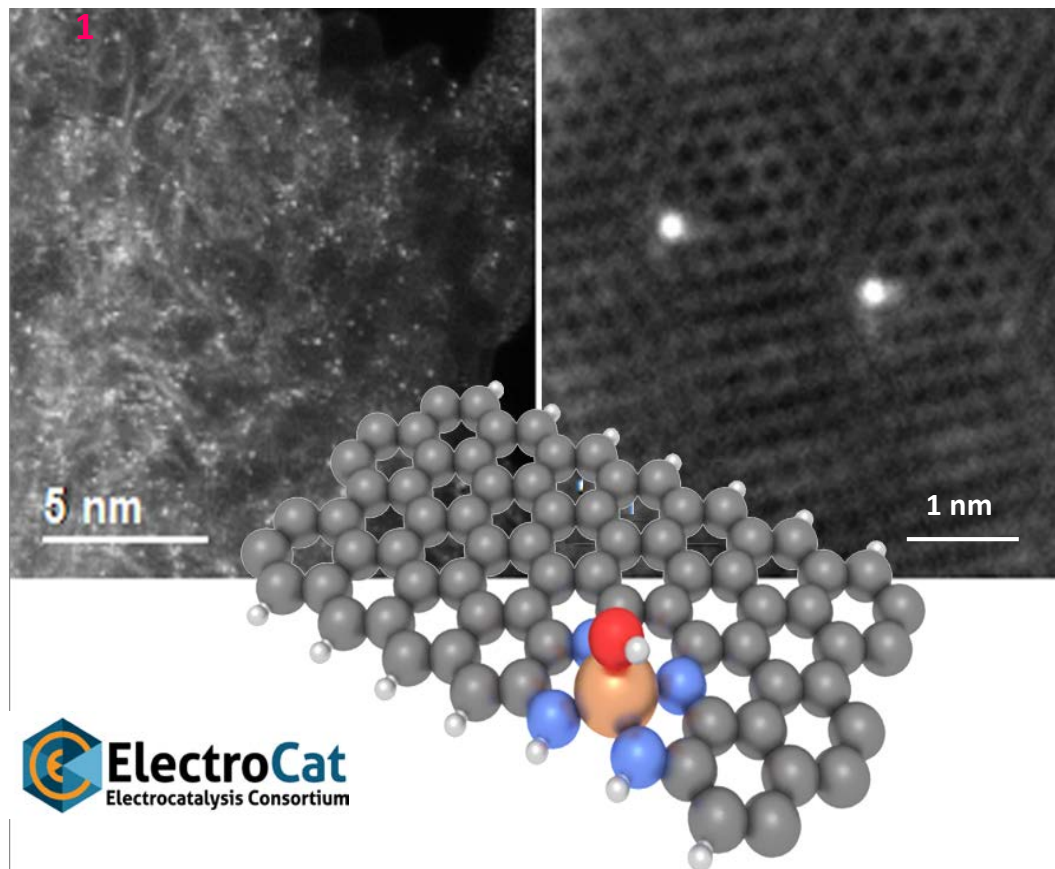
- Obtained **direct microscopic and spectroscopic evidence** of a majority of Fe sites being on the surface and **atomically dispersed** in (AD)Fe-N-C



High-Throughput (HT)

- Used HT software to calculate **durability descriptor** for PGM-free cathode catalysts
- Used HT robotic system to **synthesize and characterize** 40 variations of (AD)Fe-N-C





(N: blue, Fe: yellow, O: red, and H: white)

Scientific Achievement

Possible active site(s) in PGM-free Fe-N-C catalyst are visualized with scanning transmission electron microscopy (STEM) and computationally correlated with specific lattice-level carbon structures.

Science Paper Highlight!

- (CM+PANI)-Fe-C catalyst
- STEM imaging, quantitative EELS, and quantum chemistry calculations pointing to zigzag edge-hosted FeN₄, spontaneously ligated with OH as likely ORR-active structures.

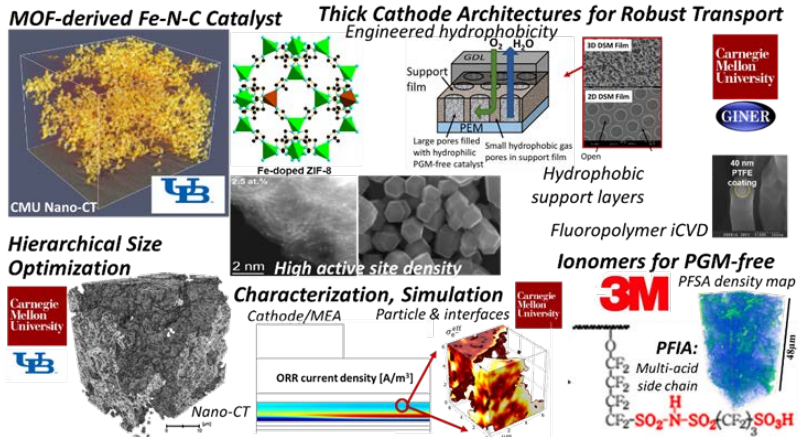
EERE Collaboration with BES: Work was performed as User Project at the Center for Nanophase Materials Sciences

H. T. Hoon, D. A. Cullen, D. Higgins, B. T. Sneed, E. F. Holby, K. L. More, and P. Zelenay, "Direct atomic-level insight into the active sites of a high-performance PGM-free catalyst," *Science* (2017). DOI: 10.1126/science.aan2255

<http://www.electrocatalysis.org/>

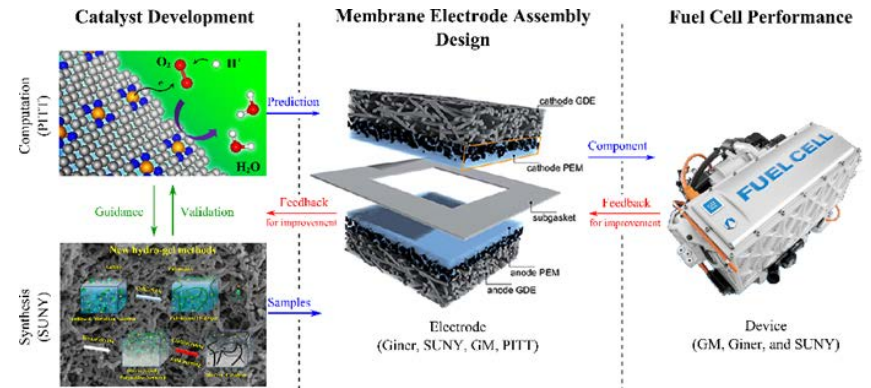
Carnegie Mellon University

Advanced PGM-free Cathode Engineering for High Power Density and Durability



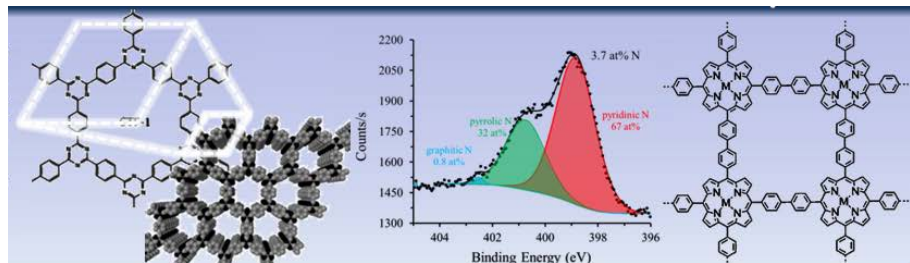
Giner Inc

Durable Mn-based PGM-Free Catalysts for Polymer Electrolyte Membrane Fuel Cells



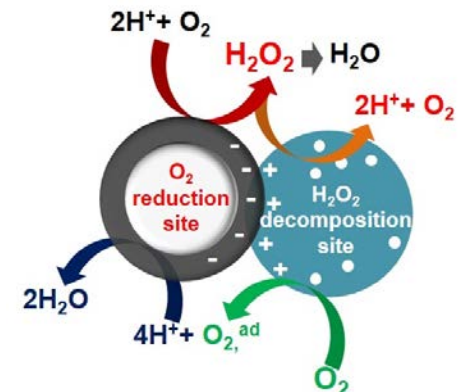
Greenway, LLC

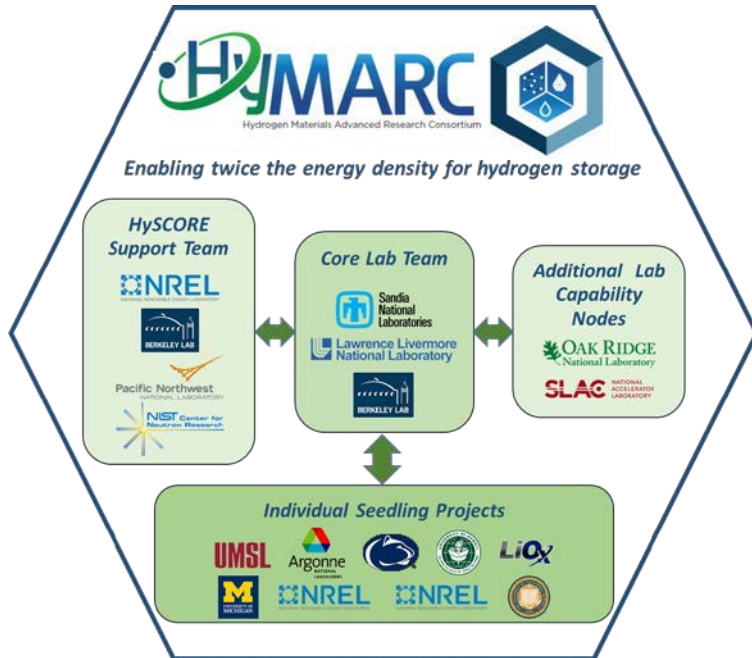
PGM-free Engineered Framework Nano Structure Catalysts



Pacific Northwest National Lab

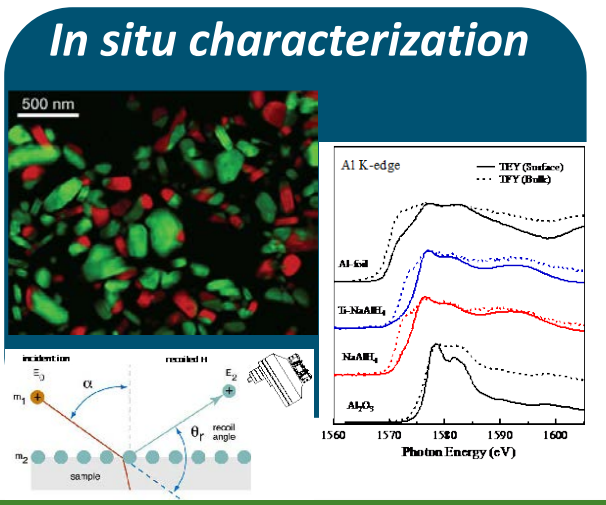
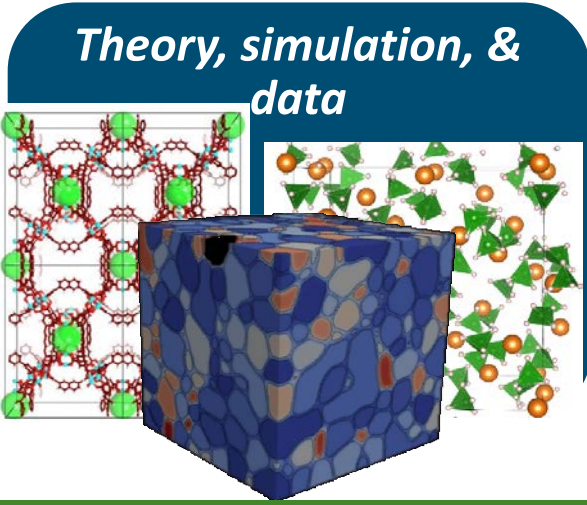
Highly Active and Durable PGM-free ORR Electrocatalysts through the Synergy of Active Sites





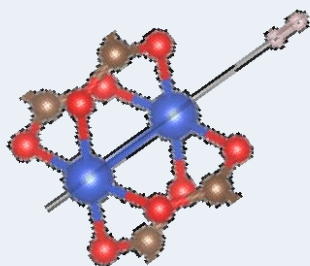
HyMARC provides capabilities & foundational understanding of phenomena governing thermodynamics & kinetics for development of solid-state H₂ storage materials

- **Delivering community tools and capabilities:**
 - **Computational models & databases** for high-throughput materials screening
 - **New characterization tools & methods** (surface, bulk, soft X-ray, synchrotron)
 - **Tailorable synthetic platforms** for probing nanoscale phenomena



HyMARC is developing extensive theoretical capabilities to facilitate materials development across all core labs & seedling projects

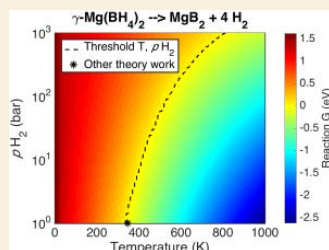
Improved sorbent isotherms



Recipes for integrating different levels of theory in sorbent isotherm models

Seedlings: PSU, NREL, UC-Berkeley

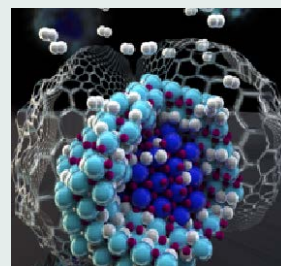
Accurate hydride thermodynamics



Finite- T free energy, environment- and morphology-dependent thermodynamics

Seedlings: ANL, U. Hawaii

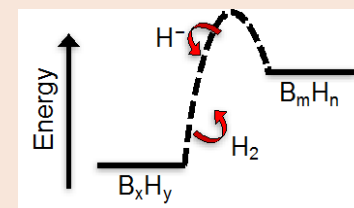
Solid mechanics & interfaces in hydrides



Internal and confinement stress effects; reactive diffuse interfaces

Seedlings: ANL, U. Hawaii, Liox, NREL

Kinetic modeling

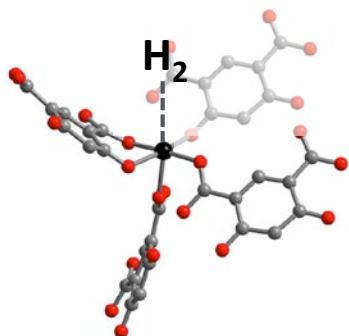


Semiempirical kinetic modeling and rate analysis; phase evolution kinetics

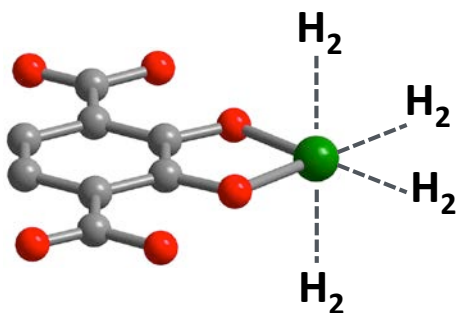
Seedlings: ANL, U. Hawaii, Liox, NREL

- ***Simulated & measured spectroscopy database (NMR, FTIR, XAS/XES) for identifying MgB_xH_y (LBNL/SNL/PNNL/NREL)***
- ***Library of analytical free energies for Li-N-H (published) & Mg-B-H (preparing manuscript), w/ validation at a range of pressures via NMR (SNL/PNNL/NREL)***
- ***Database of classical potentials for simulating borohydride mixtures & interfaces (SNL)***

Website: hymarc.org

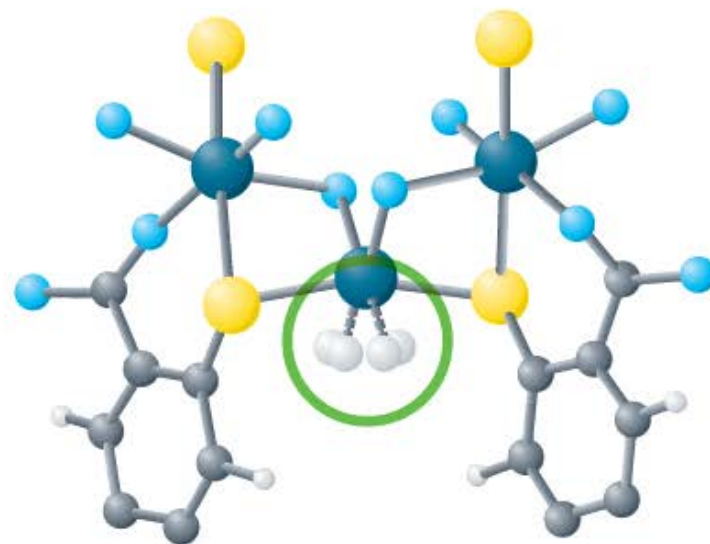
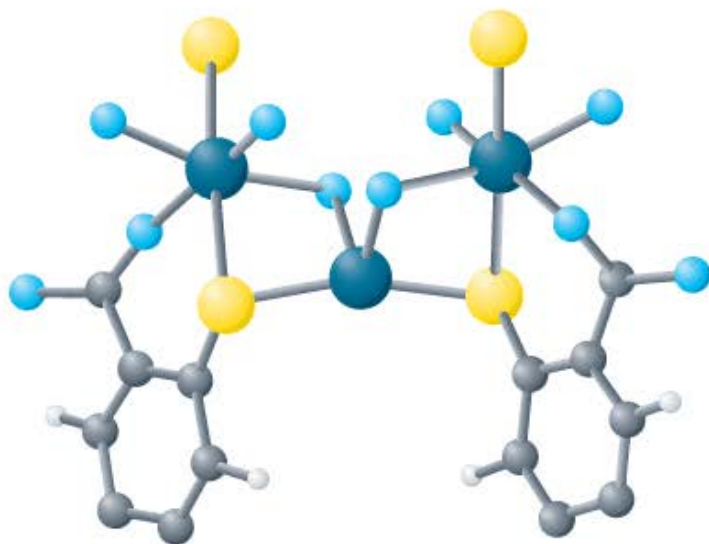


Traditional Materials:
1 H₂ per metal cation



Target Materials:
4 or more H₂ per metal cation??

- Increasing the density of adsorbed H₂ in storage materials is a major goal to enable volumetric capacities approaching DOE targets
- HyMARC groups at LBNL & NIST demonstrated two H₂ molecules bound at a single site in a metal-organic framework for the first time



- 32 - Publications published or submitted for publication**
- 4 - Patents applications submitted**
- 7 - Manuscripts in preparation as of April 2017**
- 2 - Selected as cover features**

B. C. Wood et al., *Advanced Materials Interfaces*, 2017, 4, 1600803.

E. S. Cho, J. J. Urban et al., *Small*, 2017, 13(3).

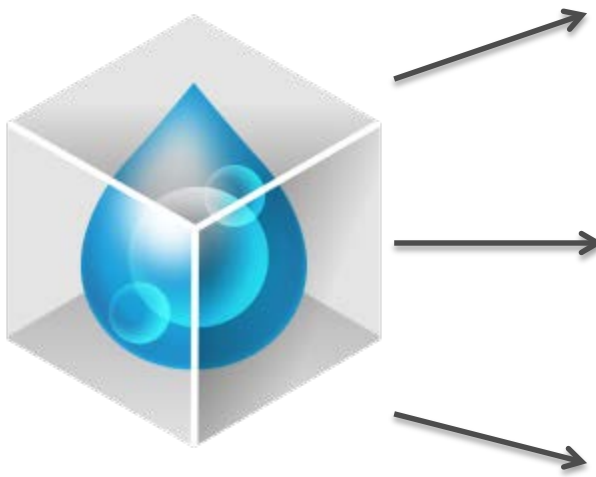
Lab teams are producing high-value R&D & disseminating it to the R&D community

Website: hymarc.org




Advanced Water-Splitting Materials (AWSM)

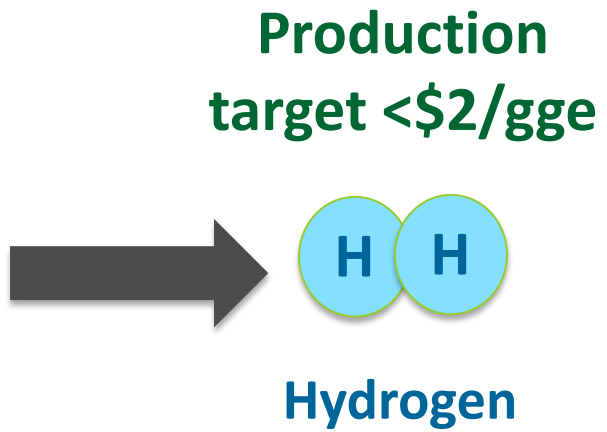


Accelerating discovery & development of innovative materials critical to advanced water splitting technologies for sustainable H₂ production, including:



Water

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



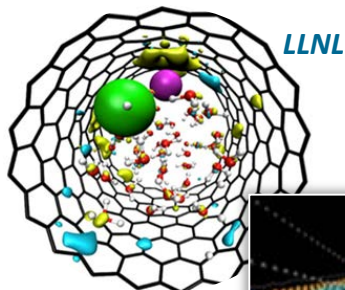
Website: h2awsm.org/



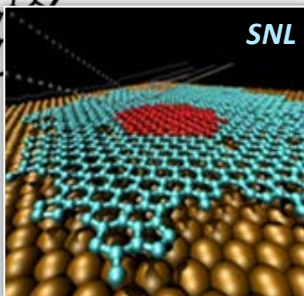
HydroGEN-AWSM Consortium

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

Materials Theory/Computation

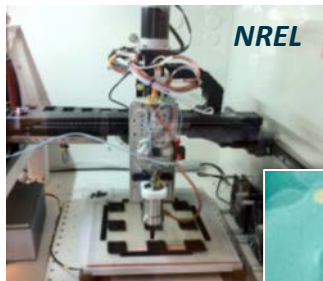


Bulk & interfacial models of aqueous electrolytes

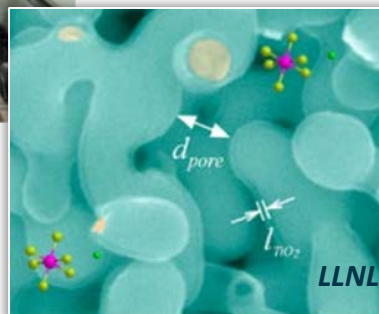


LAMMPS classic molecular dynamics modeling relevant to H_2O splitting

Advanced Materials Synthesis



High-throughput spray pyrolysis system for electrode fabrication

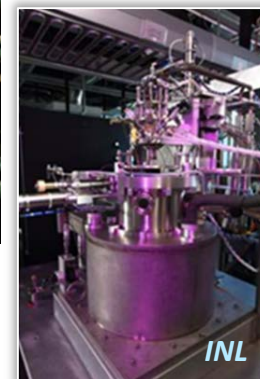


Conformal ultrathin TiO_2 ALD coating on bulk nanoporous gold

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/>



Nature Energy

Self-optimizing, highly surface-active layered metal dichalcogenide catalysts for hydrogen evolution

Yuanyue Liu^{1†‡}, Jingjie Wu^{1‡}, Ken P. Hackenberg^{1‡}, Jing Zhang¹, Y. Morris Wang², Yingchao Yang¹, Kunttal Keyshar¹, Jing Gu³, Tadashi Ogitsu², Robert Vajtai¹, Jun Lou¹, Pulickel M. Ajayan¹, Brandon C. Wood^{2*} and Boris I. Yakobson^{1*}



Steering Committee Member (Tadashi) owns a FCEV and chooses a unique license plate



High Impact Research in Photoelectrochemistry

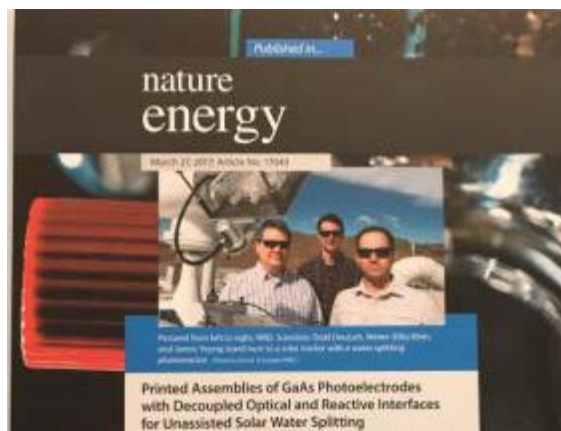
**New PEC World Record
Benchmarked at >16% STH**

Achieving Record Performance

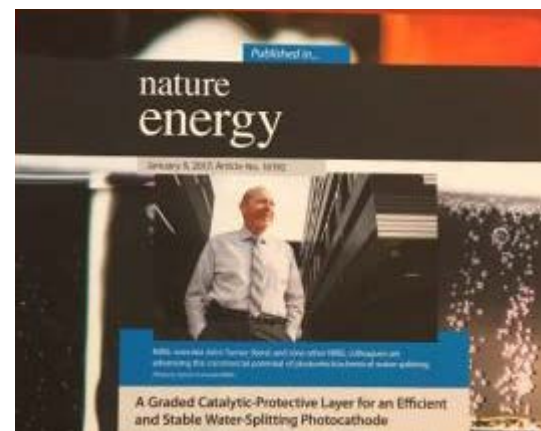
3 *Nature Energy* publications:



World-record Photoelectrolysis Efficiency with Inverted Metamorphic Multi-junction Semiconductors



Mass-spectrometer based Faradaic efficiency system



Protected Layer to Enhance Durability

- **Non-provisional patent on “PASSIVATING WINDOW AND CAPPING LAYER FOR PHOTOELECTROCHEMICAL CELLS.”** August 16, 2016 (Application No. 62/375,718).
- **Non-provisional patent on “Devices and Methods for Photoelectrochemical water splitting”** March 23rd, 2016 (Application 20160281247).
- **Record of Invention “Multiple quantum well solar cells for hydrogen generation by photoelectrochemical water splitting”** October 17, 2017.

High Impact Publications and Patent Applications



HydroGEN: Kicking Off a Nationwide R&D Effort

10 Labs
6 Companies
22 Universities





NEW HydroGEN Seedling Projects

19 Proposals Selected, Negotiated, and Awarded
44 unique capabilities being utilized across 6 core labs

Advance Electrolysis (8)

LTE (5)

HTE (3)

PEC (5)

**Benchmarking &
Protocols (1)**

STCH (5)

2-Step MO_x (4)

Hybrid cycle (1)





HydroGEN Seedling Project Example (ANL)

PGM-free OER Catalysts for Proton Exchange Membrane Electrolyzer (PEME)

Lead: Di-Jia Liu, Argonne National Laboratory

Sub: Gang Wu, U. of Buffalo, Hui Xu, Giner Inc.

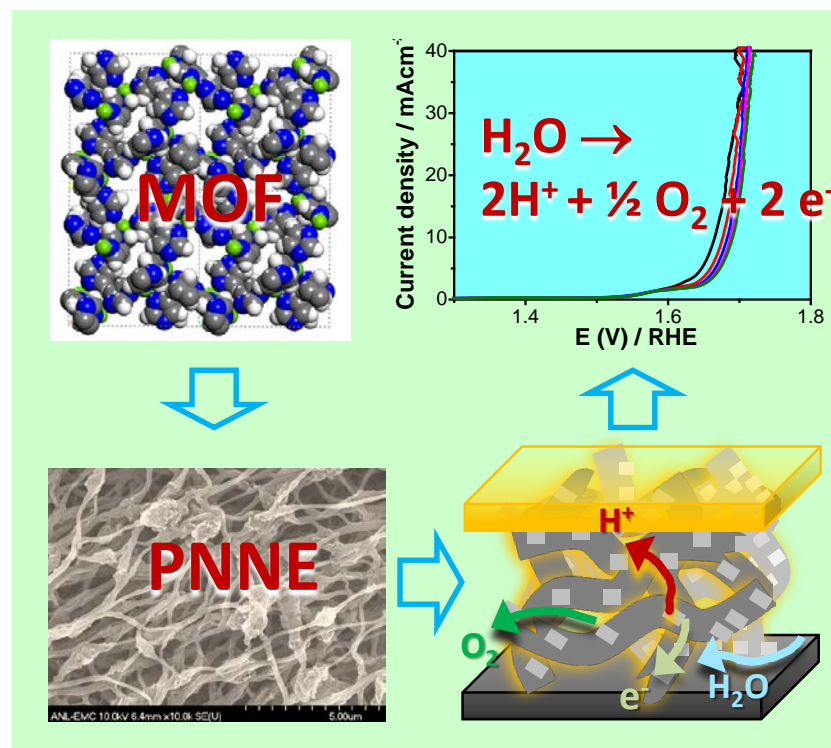
Award #	EE2.2.0.202
Year 1 Funding	\$250,000

Project Vision

To lower the capital cost of PEME by adopting precious-metal free oxygen evolution reaction (OER) electro-catalysts

Project Impact

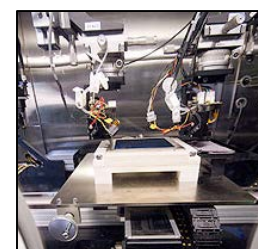
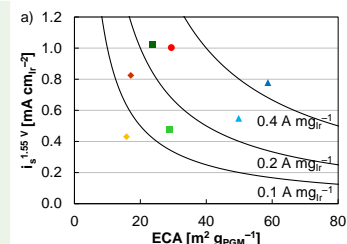
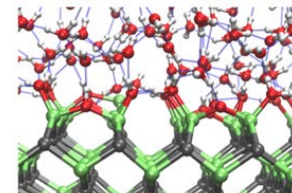
To reduce the anode catalyst cost by 20 folds by developing one or more Pt group metal (PGM) - free OER catalysts with the performance approaching to that of Ir catalyst, demonstrated at PEME level.





Effective Resource Nodes Leveraging (ANL)

National Lab	Capability	Node Role/Task
LLNL	Computational Materials Diagnostics	Predictive modeling to support better OER catalyst design
LBNL	DFT & Ab initio Calculations for Water Splitting	Improve understanding of active site structure & transition state of OER catalysis
SNL	Advanced Electron Microscopy	High resolution imaging support to better understand catalyst morphology and composition
NREL	Electrolysis Catalyst Synthesis, Ex situ Characterization	Supports catalyst performance characterization
NREL	High-throughput MEA/Electrode Development	Supports catalyst ink characterization and electrode development & testing





HydroGEN Framework and Website

From drawing-board to consortium full deployment in 6 months!



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Capabilities

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meeting the challenge

Accelerating research, development, and deployment of advanced water splitting technologies for clean, sustainable hydrogen production

Learn More

FEATURED CAPABILITY

Multiscale Modeling of Water-Splitting Devices

IN THE NEWS

Proton OnSite Announces \$1.8 Million Award to Lead Advanced Water...

Visit the HydroGEN website at <https://www.h2awsm.org>



HydroGEN Steering Committee



Huyen Dinh
(Director)



Adam Weber
(Deputy Director)



Anthony McDaniel
(Deputy Director)



Richard Boardman



Tadashi Ogitsu



Héctor Colón-Mercado



Eric Miller and Katie Randolph, FCTO



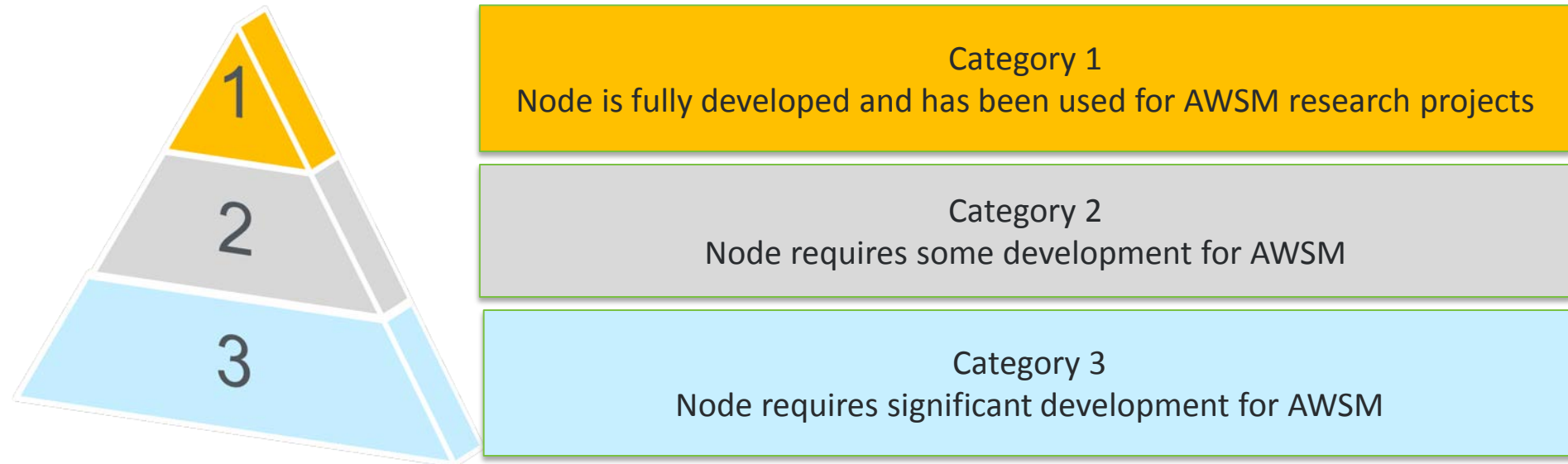


Steering Committee's Node Evaluation Process

Capability Node Evaluation Process:

- **Relevant** to water splitting pathways (AE, PEC, STCH)
- **Available** resources and associated expert(s) to support the capability and available to external stakeholders
- **Unique** to the national laboratory system and comprise expertise, tools, and techniques

Node Readiness Category Chart



Category refers to availability, readiness, and relevance to AE, PEC, STCH and not necessarily the expense and time commitment



User-Friendly Node Search Engine for Stakeholders

LIST OF CAPABILITIES

[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)

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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

Advanced Water-Splitting Materials Requirements Based on Flowsheet Development and Techno-Economic A...

SRNL HT 1, HTE 1, STCH 2, LTE 3, PEC 3

Albany: Open-Source Multiphysics Research Platform

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

ALD Based Surface Functionalization and Porosity Control

LLNL PEC 3

Analysis and Characterization of Hydrided Material Performance

INL HTE 2

Beyond-DFT Simulation of Energetic Barriers and Photoexcited Dynamics

LLNL PEC 2

Cascading Pressure Reactor

SNL STCH 1





HydroGEN Data Hub: Making digital data accessible

- Secure Project space for Team members
- Create Datasets and Upload files
- View and Download Project Data

- Metadata tools to support Advanced Search
- Link to other data repositories or databases
- Data Plug-ins for visualization and graphing of data



Log In Register

Home Projects Data About

HydroGEN Data Hub

The submission point for data collected from research conducted by the Advanced Water Splitting Materials National Laboratory Consortium



Register

Request a HydroGEN account.



Discover

Search the repository.



Submit Data

Upload and archive your data.
Share data with others.



HydroGEN Data Hub currently has 112 users,
26 Projects, 84 Datasets, 97 Resources

HydroGEN Data Hub Home Page
(<https://datahub.h2awsm.org/>)





Technology Transfer Activities

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 (nearly complete)

- Developed and finalized a catalog of pre-approved, mutual agreements between all consortium partners
- Facilitate rapid IP, NDA, and contract agreements
- Executed all 19 project NDAs





Establishing Best Practices & Benchmarking

Benchmarking Advanced Water Splitting Technologies

PI: Kathy Ayers, Proton OnSite

Co-PIs: Ellen B. Stechel, ASU;

Olga Marina, PNNL;

CX Xiang, Caltech

Consultant: Karl Gross

- Develop standardized Best Practices for characterizing & benchmarking AWSMs
- Foundation for accelerated materials RD&D for broader AWS community
- ***Extensive collaboration & engagement with HydroGEN***

Zhebo Chen, Huyen Dinh,
and Eric Miller

Photoelectrochemical Water Splitting

Standards,
Experimental
Methods, and
Protocols

30,000
Downloads to
date

*Examples of Best
Practices & Protocols*

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eBooks in the
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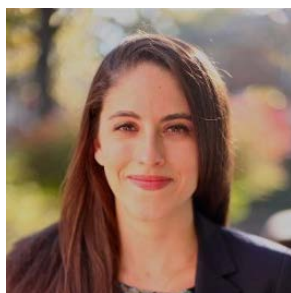
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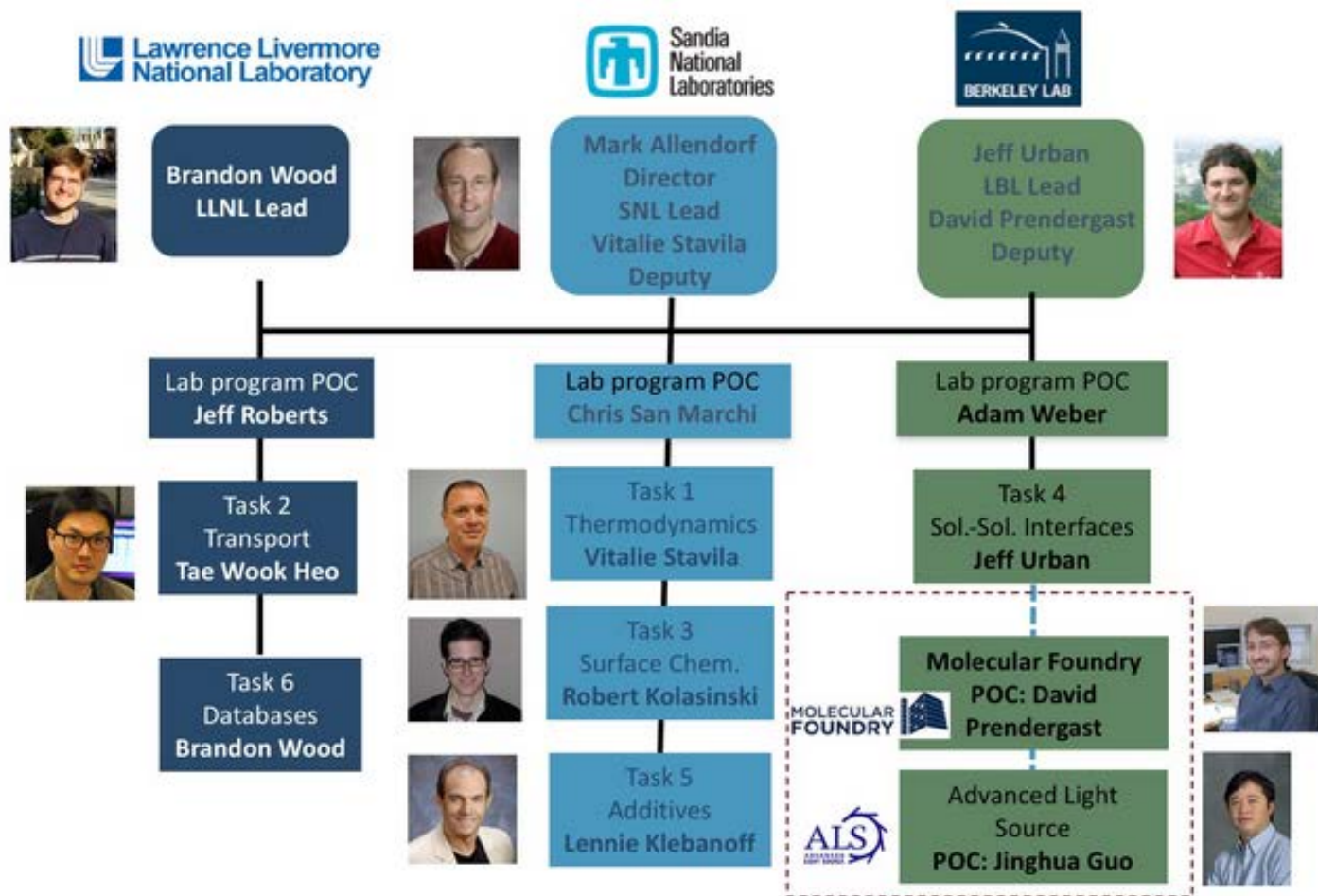
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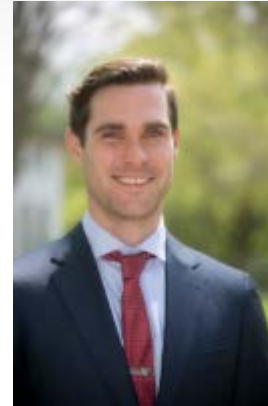
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Thank You for Your Attention