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

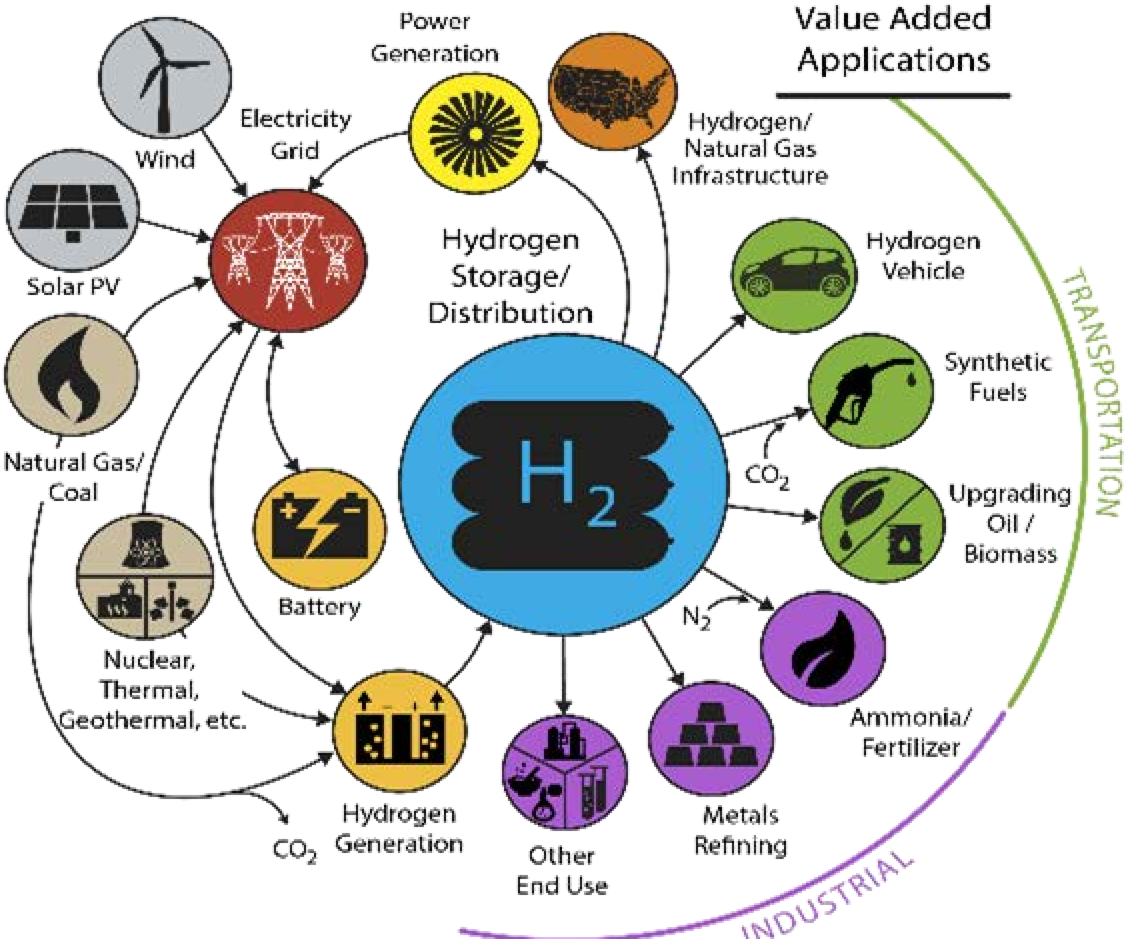
Date: 2/14/2018

Venue: 2018 DOE Hydrogen and Fuel Cell Technical Advisory Committee

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

H2@Scale Energy System Vision

Transportation & Beyond



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

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

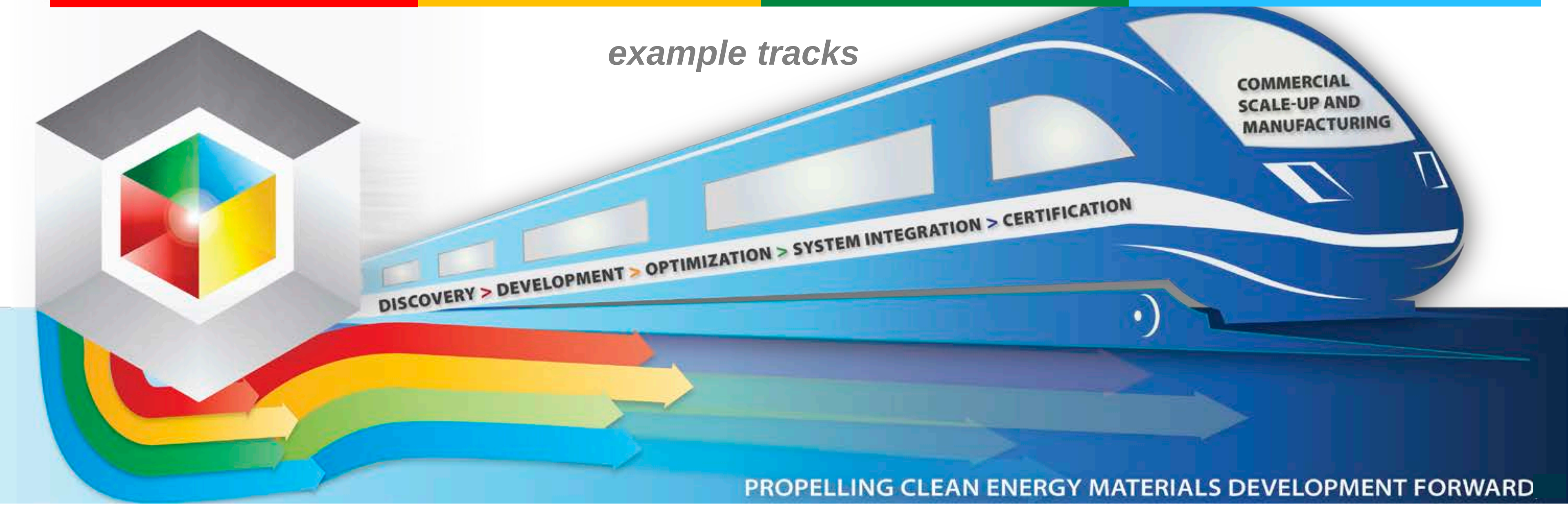
https://energy.gov/eere/fuelcells/h2-scale

Energy Materials Network (EMN)

Energy Materials Network
U.S. Department of Energy

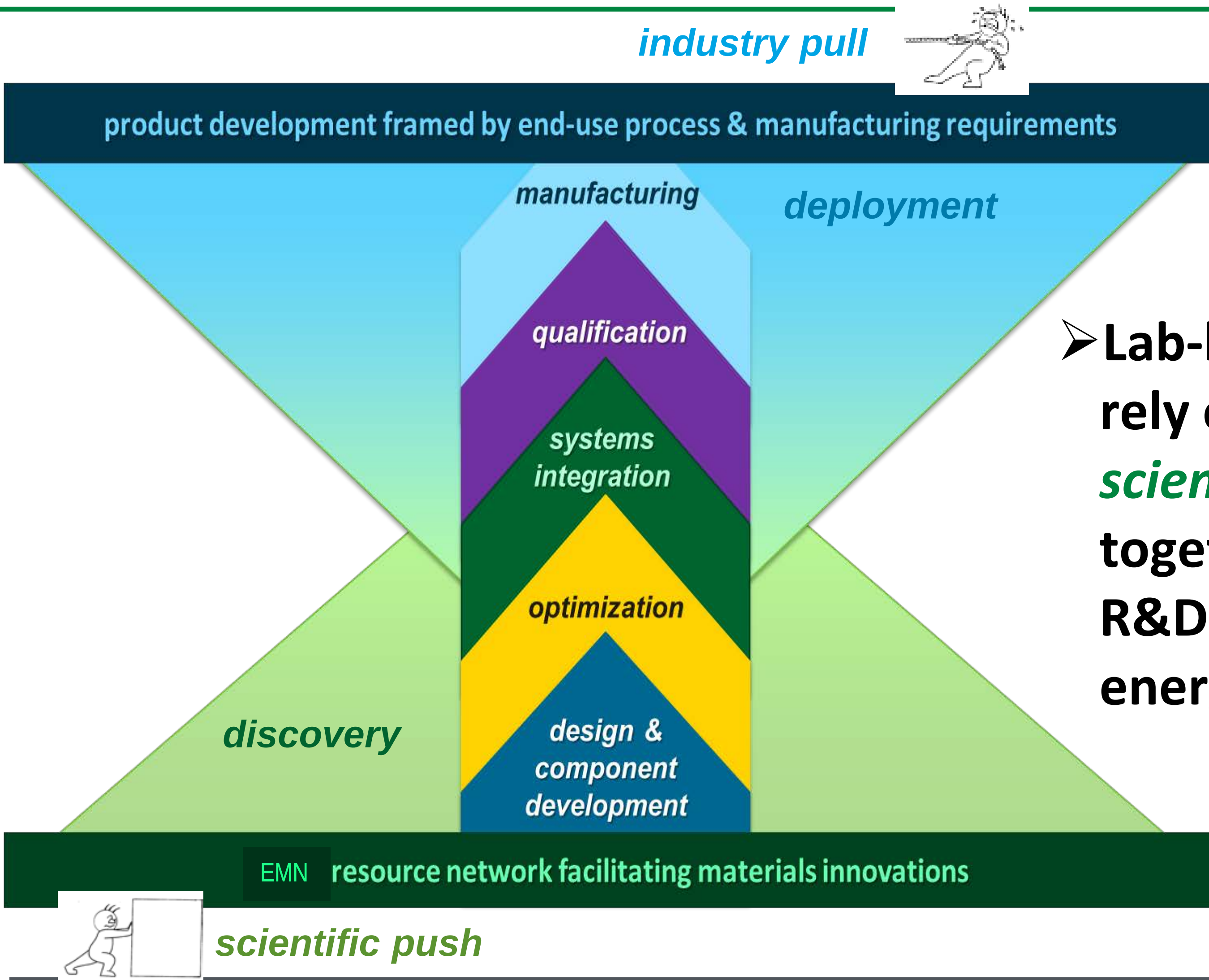
DOE's EMN aims to accelerate early-stage applied R&D in materials tracks aligned with some of the nation's most pressing sustainable energy challenges

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



- 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

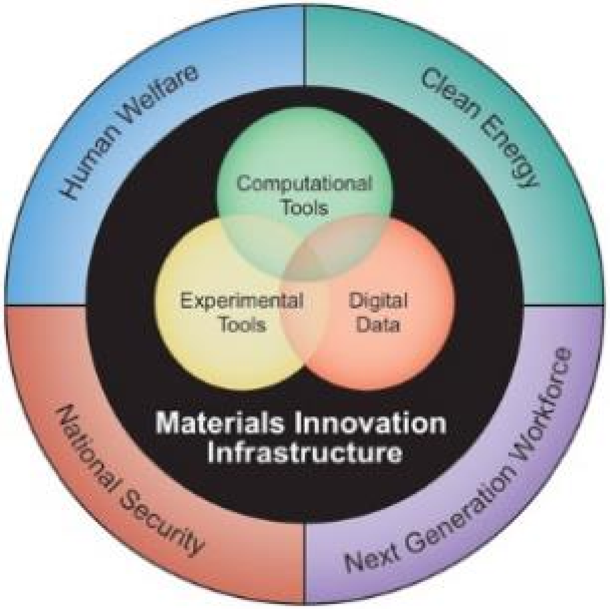
Foundation in Modern Materials R&D

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

- CaloriCool™ – Caloric Materials Consortium
- ChemCatBio – Chemical Catalysis for Bioenergy
- DuraMAT – Durable Module Materials Consortium
- ElectroCat – Electrocatalysis Consortium
- HydroGEN – Advanced Water Splitting Materials
- HyMARC – Hydrogen Materials Advanced Research Consortium
- LightMAT – Lightweight Materials Consortium

Seven EMN consortia have been successfully deployed to date

ElectroCat: PGM-Free Fuel Cell Electrocatalysts

ElectroCat
Electrocatalysis Consortium

Core Labs

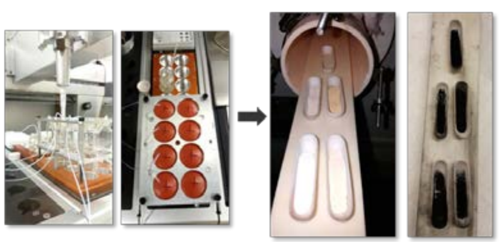
Los Alamos National Laboratory · Argonne National Laboratory · Oak Ridge National Laboratory · NREL

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

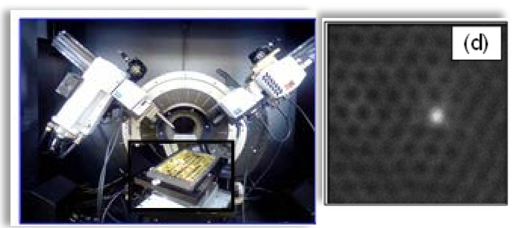
➢ ***Comprising 27 world-class capabilities and expertise in:***

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

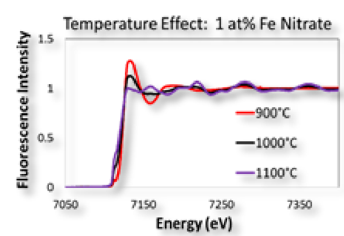
Synthesis, Processing and Manufacturing



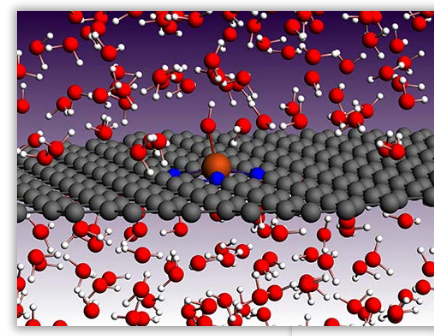
Characterization and Synthesis

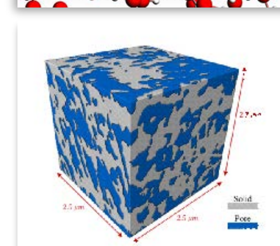


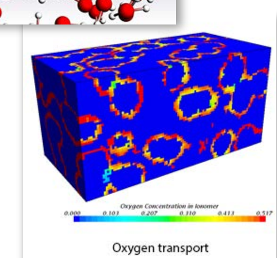
Fe K-Edge EXAFS



Computation, Modeling & Data Management







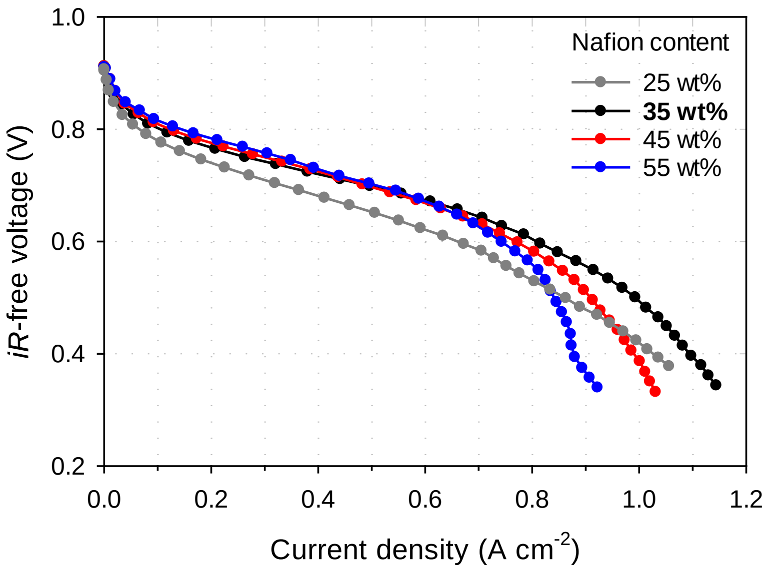
Website: electrocat.org

ElectroCat Accomplishments in ORR Activity

Performance Improvement

- Improved PGM-free H_2-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 H_2, 200 sccm, 1.0 bar H_2 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



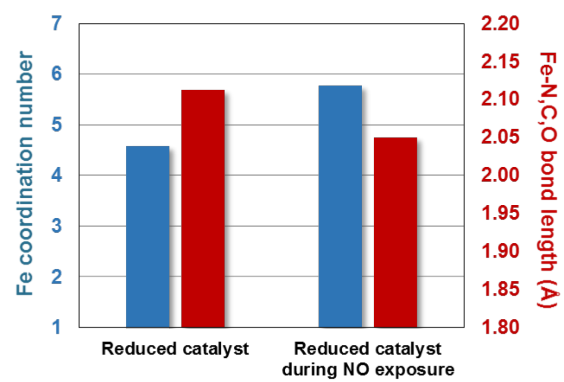
- Increased ORR activity for atomically-dispersed Fe-N-C catalyst **by 20 mV** at ***E*$_{½}$**

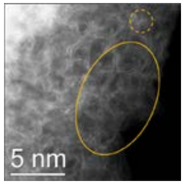
http://www.electrocat.org/

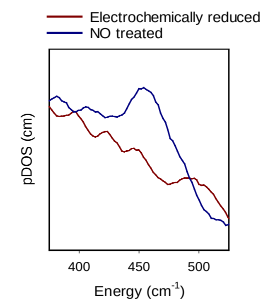
ElectroCat Electrocatalysis Consortium

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**

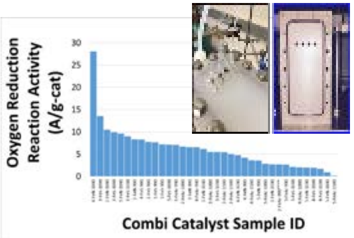




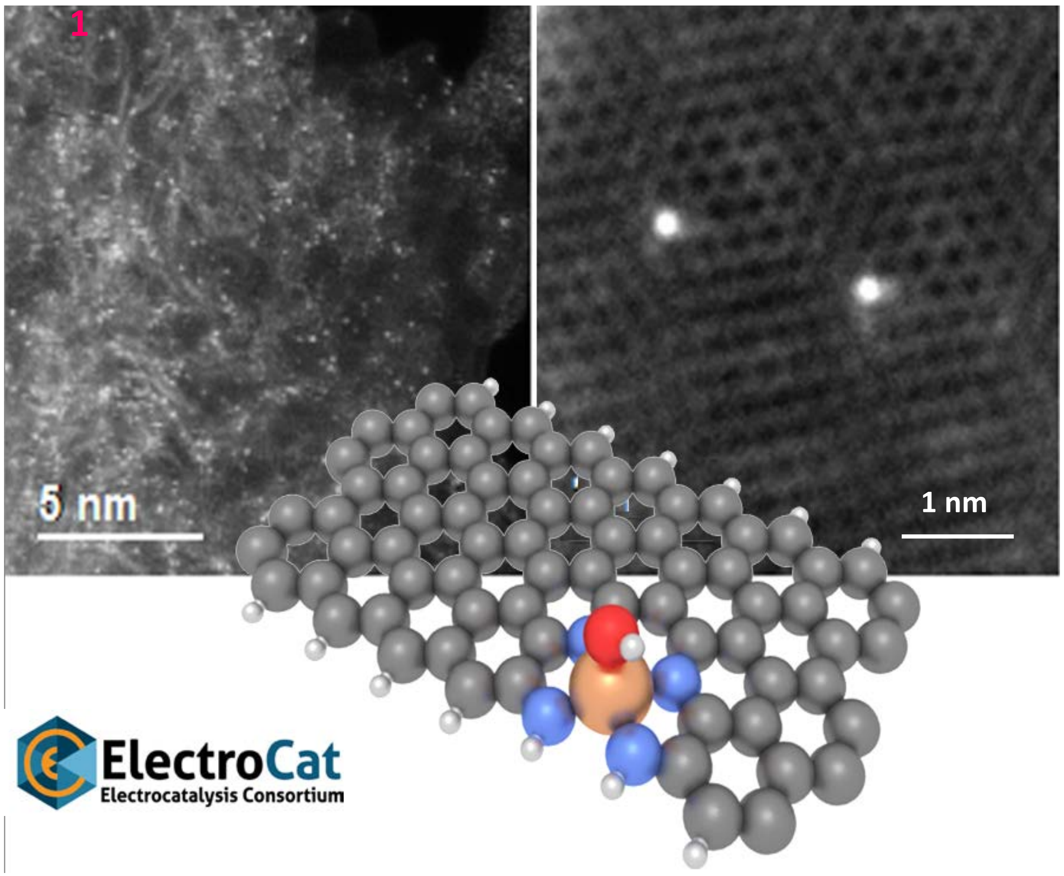


High-Throughput (HT)

- 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



In Pursuit of Active Sites in PGM-Free Catalysts



(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 FeN_4, 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

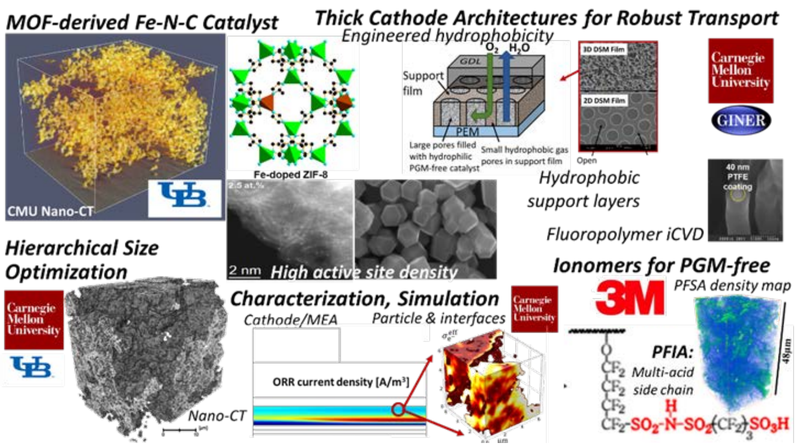
H. T. Hoon, D. A. Cullen, D. Higgins, B. T. Sneed, E. F. Holby, K. L. More, and P. Zelenay, "Direct atomic-level insight into the active sites of a high-performance PGM-free catalyst," *Science* (2017). DOI: 10.1126/science.aan2255

http://www.electrocat.org/

FOA Projects added to ElectroCat in FY17

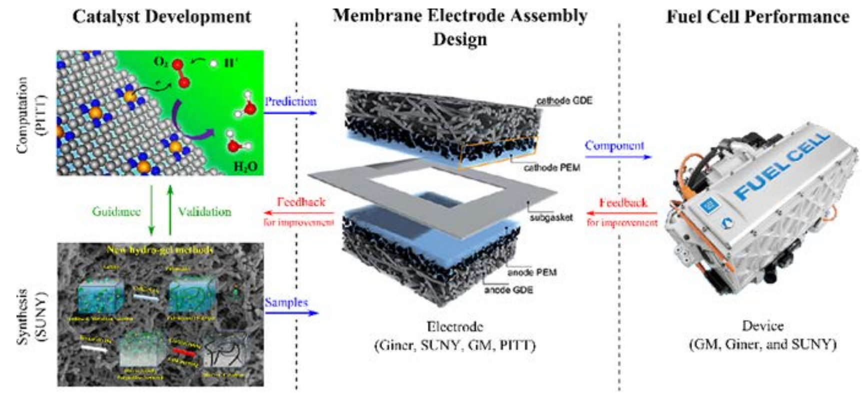
Carnegie Mellon University

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



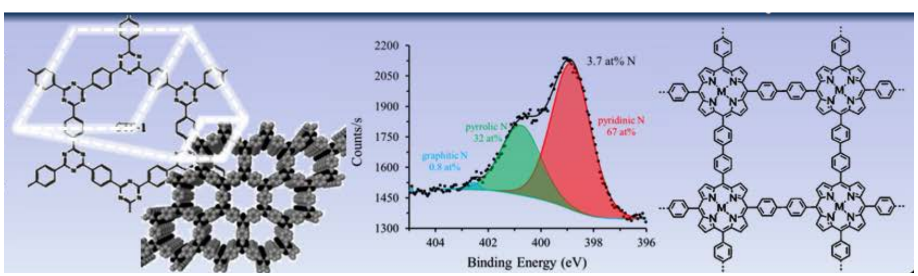
Giner Inc

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



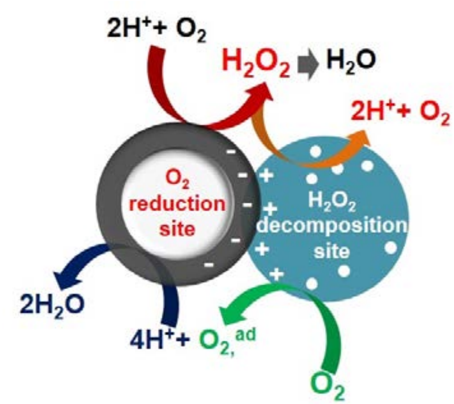
Greenway, LLC

PGM-free Engineered Framework Nano Structure Catalysts

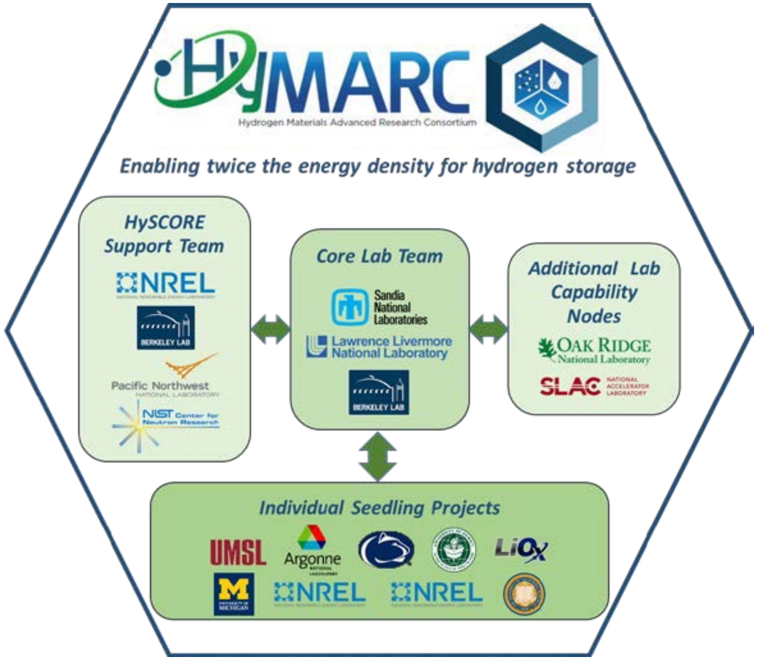


Pacific Northwest National Lab

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



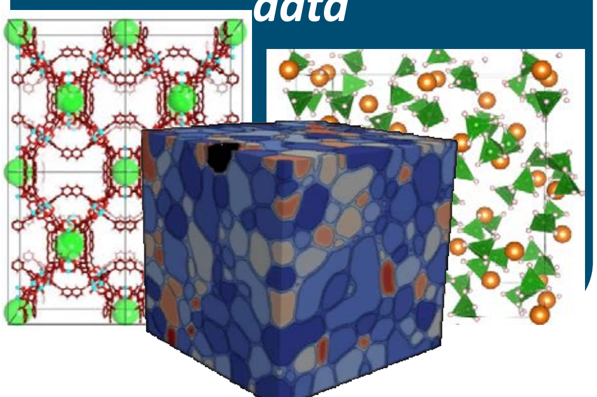
Breakthrough H_2 Storage Materials



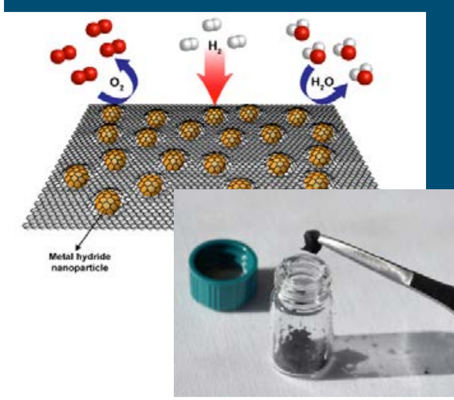
HyMARC provides capabilities & foundational understanding of phenomena governing thermodynamics & kinetics for development of solid-state H_2 storage materials

- **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

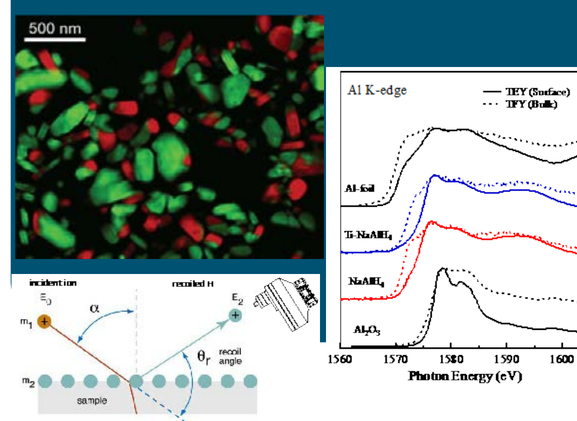
Theory, simulation, & data



Controlled synthesis



In situ characterization

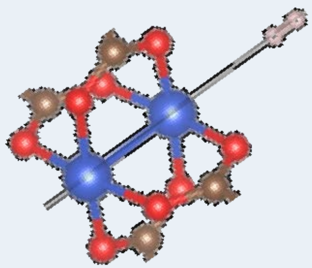


Website: hymarc.org

Technical Accomplishments

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

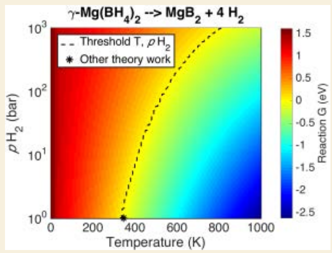
Improved sorbent isotherms



Recipes for integrating different levels of theory in sorbent isotherm models

Seedlings: PSU, NREL, UC-Berkeley

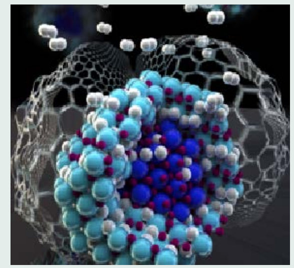
Accurate hydride thermodynamics



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

Seedlings: ANL, U. Hawaii

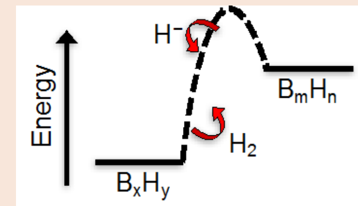
Solid mechanics & interfaces in hydrides



Internal and confinement stress effects; reactive diffuse interfaces

Seedlings: ANL, U. Hawaii, Liox, NREL

Kinetic modeling



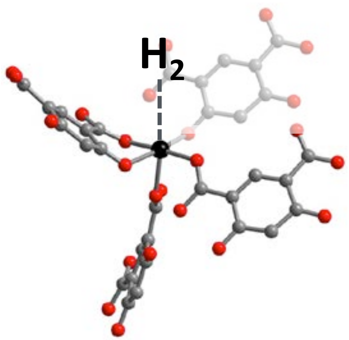
Semiempirical kinetic modeling and rate analysis; phase evolution kinetics

Seedlings: ANL, U. Hawaii, Liox, NREL

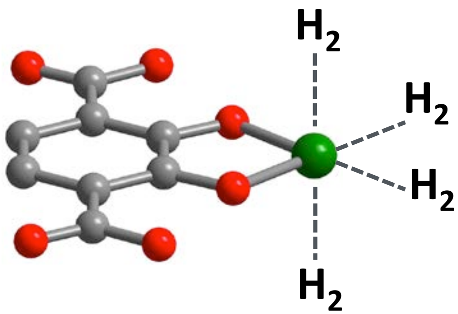
- ***Simulated & measured spectroscopy database (NMR, FTIR, XAS/XES) for identifying MgB_xH_y (LBNL/SNL/PNNL/NREL)***
- ***Library of analytical free energies for Li-N-H (published) & Mg-B-H (preparing manuscript), w/ validation at a range of pressures via NMR (SNL/PNNL/NREL)***
- ***Database of classical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

Website: hymarc.org

Technical Accomplishments

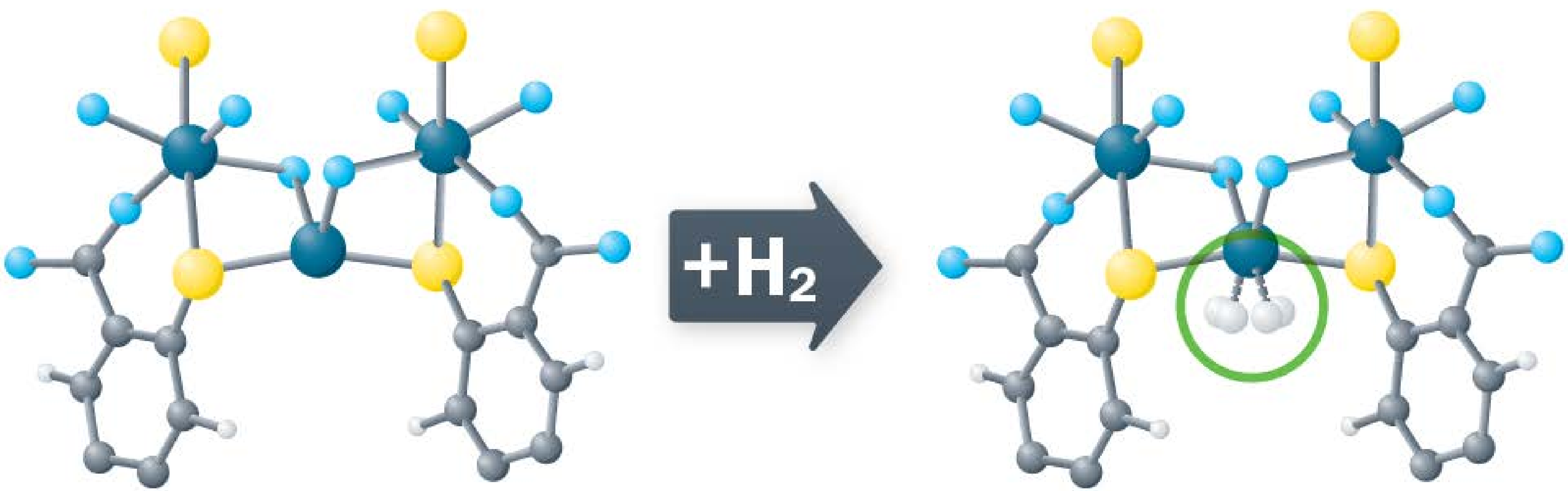


Traditional Materials:
1 H_2 per metal cation



Target Materials:
4 or more H_2 per metal cation??

- **Increasing the density of adsorbed H_2 in storage materials is a major goal to enable volumetric capacities approaching DOE targets**
- **HyMARC groups at LBNL & NIST demonstrated two H_2 molecules bound at a single site in a metal-organic framework for the first time**



Website: hymarc.org

Accomplishments & Publications

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)

HydroGEN
Advanced Water Splitting Materials

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

Accelerating discovery & development of innovative materials critical to advanced water splitting technologies for sustainable H_2 production, including:

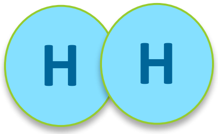
Water

Photoelectrochemical (PEC)

Solar Thermochemical (STCH)

Low- and High-Temperature Advanced Electrolysis (LTE & HTE)

Production target <$2/gge



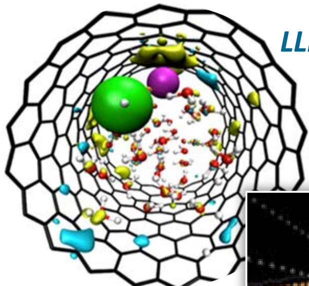
Hydrogen

Website: h2awsm.org/

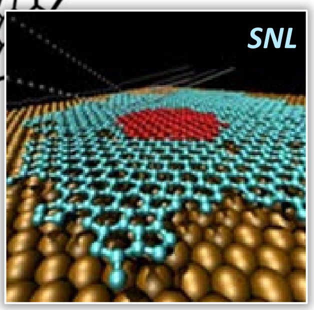
HydroGEN-AWSM Consortium

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

Materials Theory/Computation

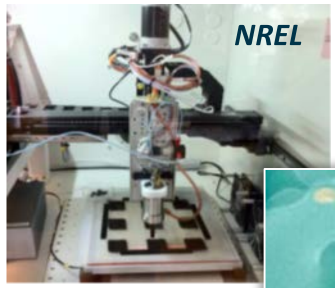


Bulk & interfacial models of aqueous electrolytes

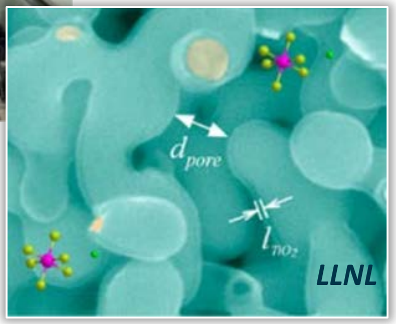


LAMMPS classic molecular dynamics modeling relevant to H_2O splitting

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/

High-Impact Computational Research in Catalysis

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 Zhang[1], Y. Morris Wang[2], Yingchao Yang[1], Kunttal Keyshar[1], Jing Gu[3], Tadashi Ogitsu[2], Robert Vajtai[1], Jun Lou[1], Pulickel M. Ajayan[1], 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

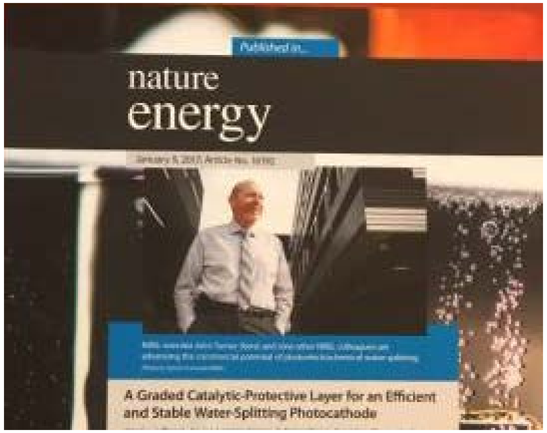
New PEC World Record Benchmarked at >16% STH

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 photolectrochemical water splitting**" October 17, 2017.

High Impact Publications and Patent Applications

HydroGEN: Kicking Off a Nationwide R&D Effort

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.

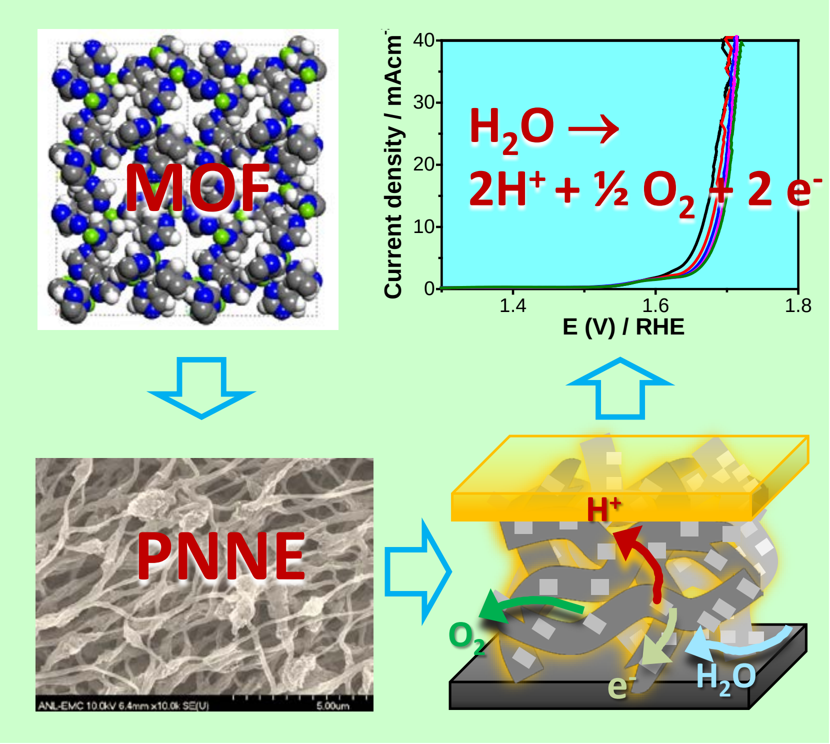
Award #	EE2.2.0.202
Year 1 Funding	$250,000

Project Vision

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

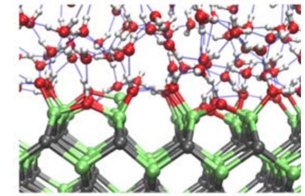
Project Impact

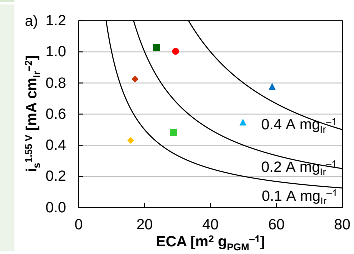
To reduce the anode catalyst cost by 20 folds by developing one or more Pt group metal (PGM) - free OER catalysts with the performance approaching to that of Ir catalyst, demonstrated at PEME level.

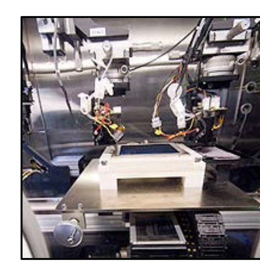


Effective Resource Nodes Leveraging (ANL)

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

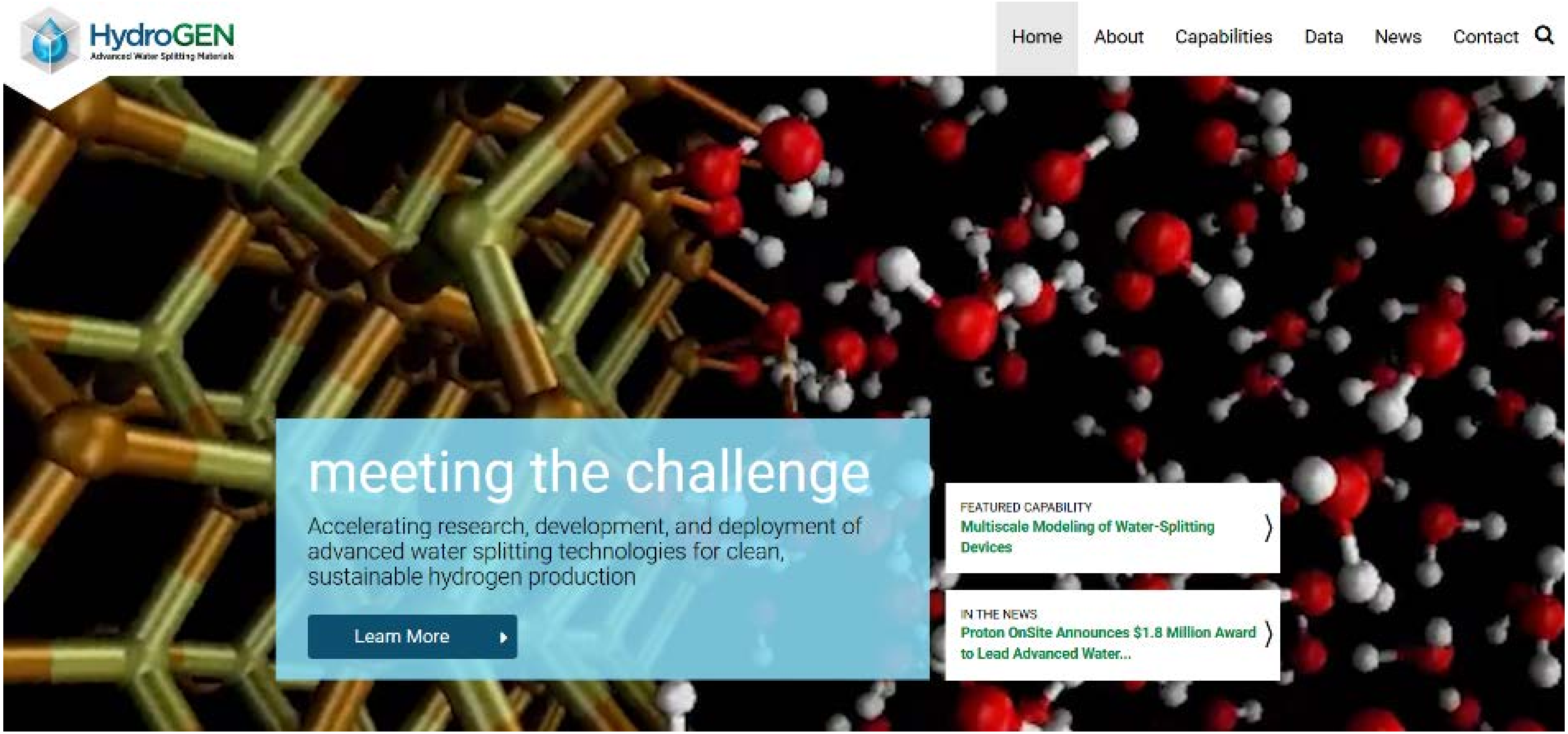






HydroGEN Framework and Website

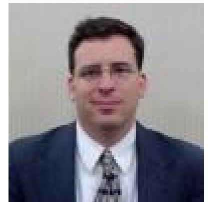
From drawing-board to consortium full deployment in 6 months!



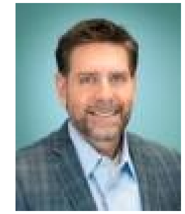
Visit the HydroGEN website at https://www.h2awsm.org

HydroGEN Steering Committee

Huyen Dinh
(Director)



Adam Weber
(Deputy Director)



Anthony McDaniel
(Deputy Director)

Richard Boardman

Tadashi Ogitsu

Héctor Colón-Mercado

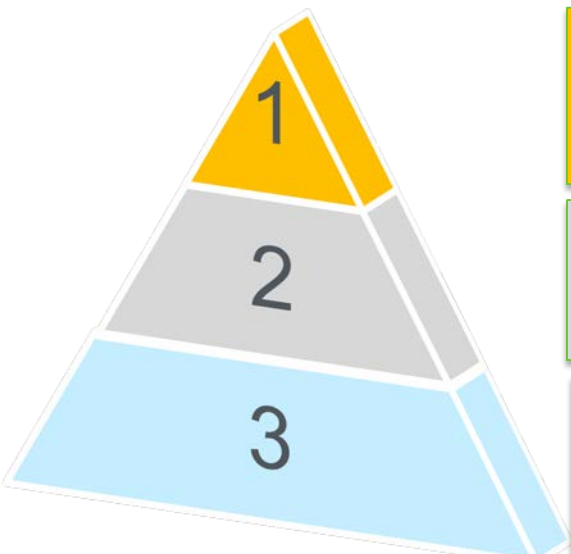
Eric Miller and Katie Randolph, FCTO

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 1
Node is fully developed and has been used for AWSM research projects

Category 2
Node requires some development for AWSM

Category 3
Node requires significant development for AWSM

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

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)

Show

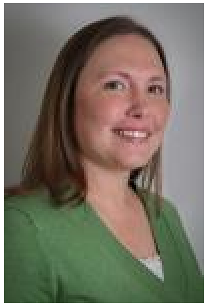
12 Apply

Reset

Showing 1 to 12 of 82 entries

1 2 3 4 Next

Capability	Lab	Technology
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

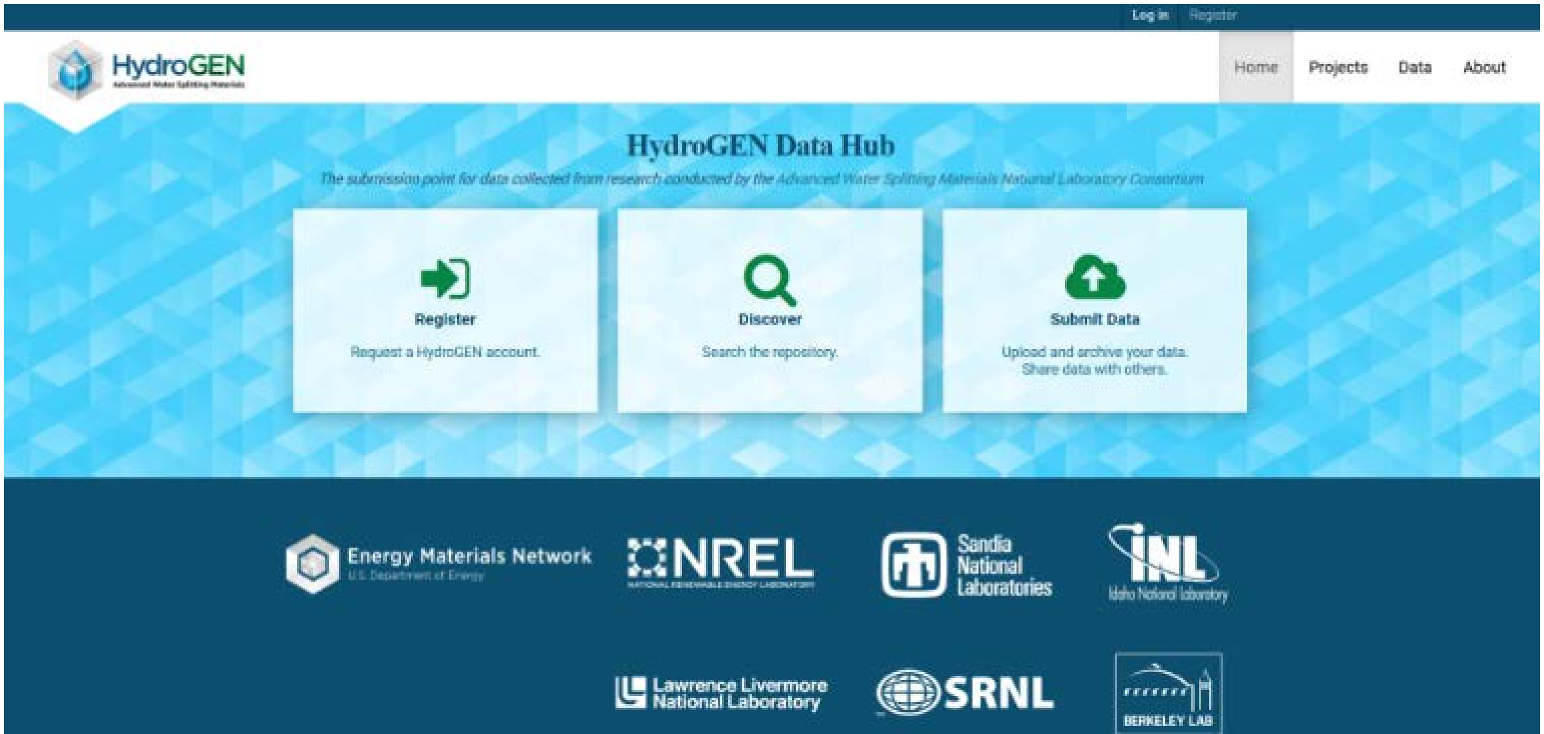


https://www.h2awsm.org/index.html

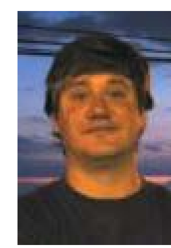
HydroGEN Data Hub: Making digital data accessible

- 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

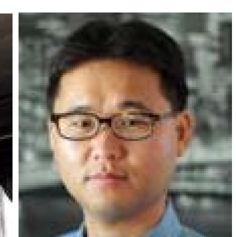





HydroGEN Data Hub currently has 112 users, 26 Projects, 84 Datasets, 97 Resources

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

Materials Transfer Agreement (MTA)
- Freedom to Operate

Cooperative Research and Development Agreement (CRADA)
- Collaboration (nearly complete)

➢ **Streamlined Access**

- ➢ 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

Top 25% most downloaded eBooks in the SpringerLink eBook Collection in 2016.

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

Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

We are at a *TURNING POINT* in History

Unlocking Hydrogen's Potential is a Critical Key to Our Sustainable Future

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

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Website: https://www.electrocat.org/

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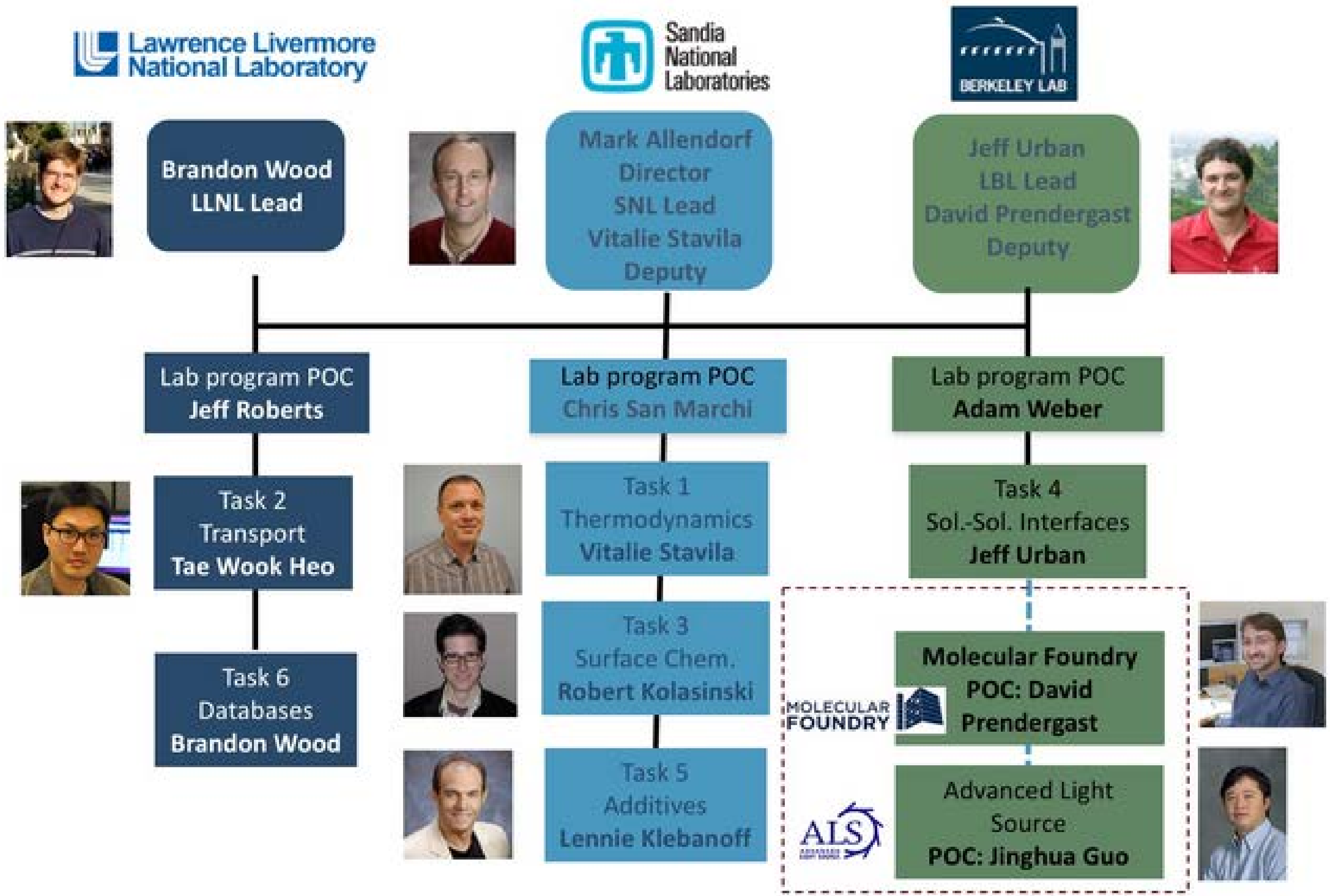

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Energy Materials Network
U.S. Department of Energy

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Advanced Water Splitting Materials

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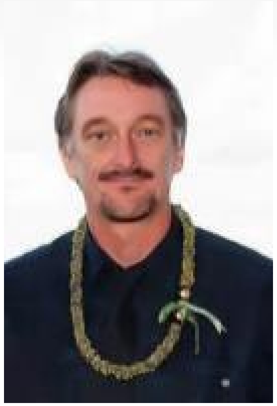
James Vickers



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Fuel Cell Technologies Office

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Advanced Water Splitting Materials

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HydroGEN
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Thank You for Your Attention