



# HydroGEN: A Consortium on Advanced Water Splitting Materials

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Presenter: Huyen Dinh, NREL

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Project ID # PD148

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# HydroGEN Overview

## Timeline and Budget

- Start date (launch): **June 2016**
- FY17 DOE funding: **\$3.6M**
- FY18 planned DOE funding: **\$6.2M**
- Total DOE funding received to date: **\$11.6M**

## Barriers

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

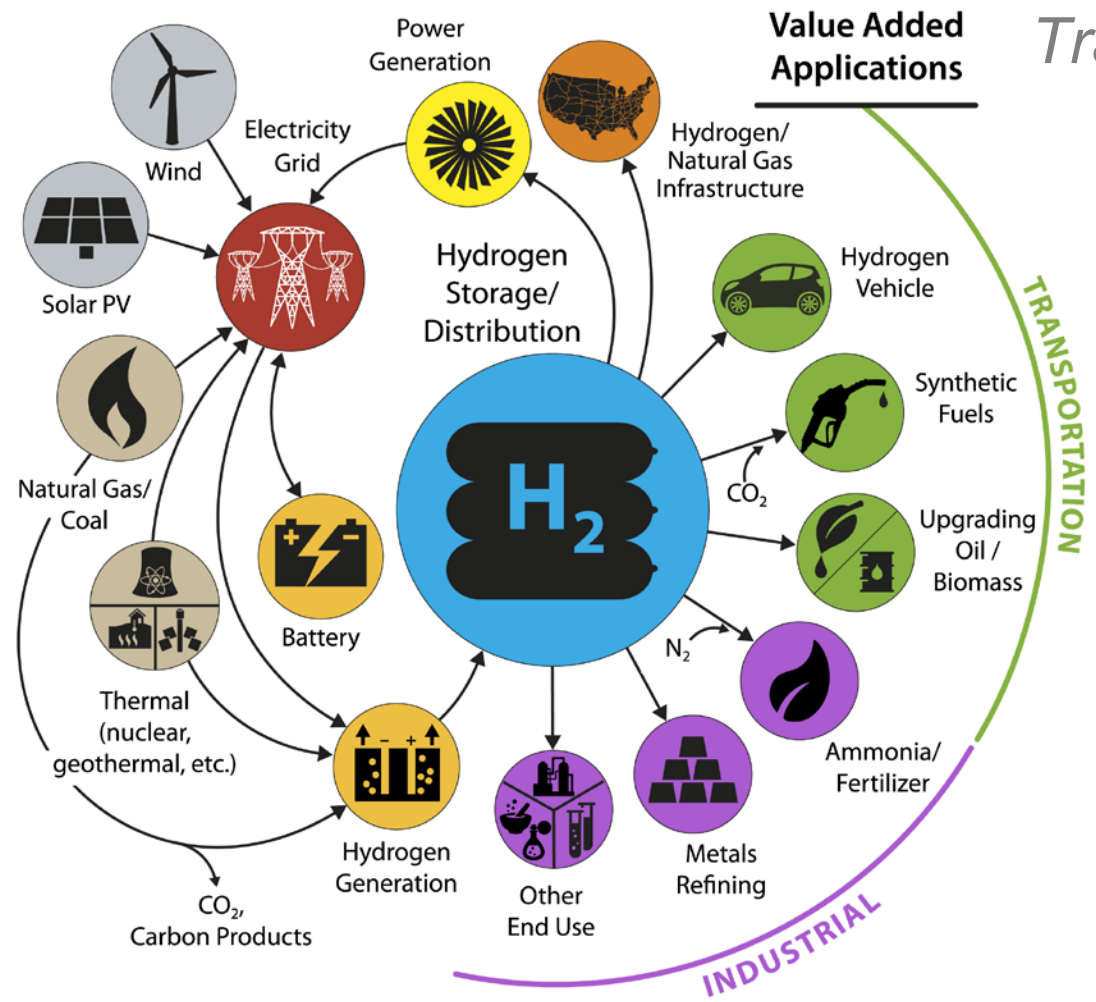
## Partners





# H2@Scale Energy System Vision

## Relevance and Impact



### 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)

## 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

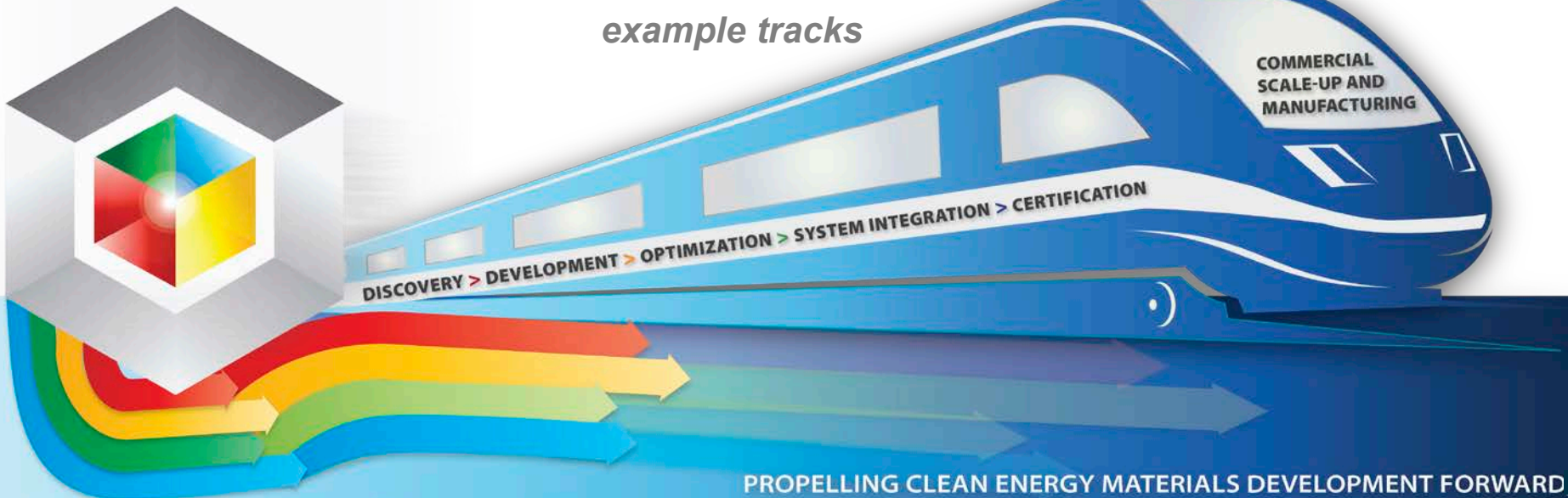
Lightweight Materials  
for Vehicles

Breakthrough  
Hydrogen Storage  
Materials

Advanced Water  
Splitting Materials for  
Hydrogen Production

Next-Generation Electro-  
catalysts for Fuel Cells

*example tracks*



*Accelerating early-stage materials R&D for energy applications*



# Relevance/Approach – Four Pillars of EMN Consortia

## World Class Materials Capability Network

Portfolio of  
unique and  
accessible  
capabilities

Access to  
leading  
technical  
expertise

## Clear Point of Engagement

Concierge,  
website,  
technology  
experts

Facilitate  
efficient  
access

## Data and Tool Collaboration Framework

Data Hub for  
public or  
secure data  
storage and  
exchange

Data expert  
support

Accessible  
digital data

## Streamlined Access

Pre-approved  
mutual  
agreements

Facilitate  
rapid IP, NDA,  
and contract  
agreements



# Advanced Water-Splitting Materials (AWSM) Relevance, Overall Objective, Impact, and Approach

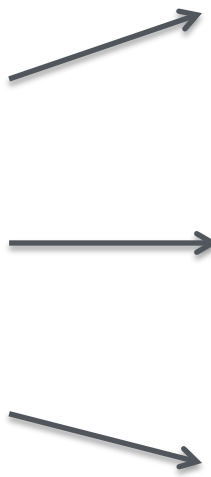
**AWSM Consortium  
Six Core Labs:**





**Accelerating R&D** of innovative materials critical to advanced water splitting technologies for clean, sustainable, and low cost H<sub>2</sub> production, including:




**Water**



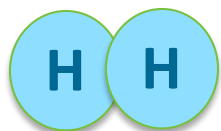
  
Photoelectrochemical (PEC)

  
Solar Thermochemical (STCH)

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



**Production target <\$2/gge**



**Hydrogen**

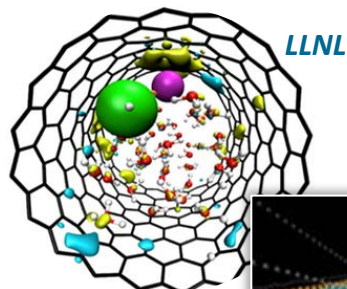


# HydroGEN-AWSM Consortium

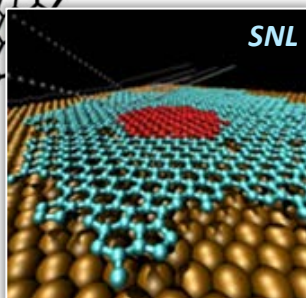
## Relevance, Overall Objective, Impact, and Approach

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

### Materials Theory/Computation

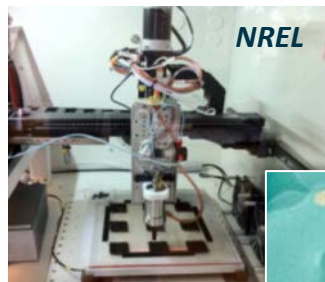


Bulk & interfacial models of aqueous electrolytes

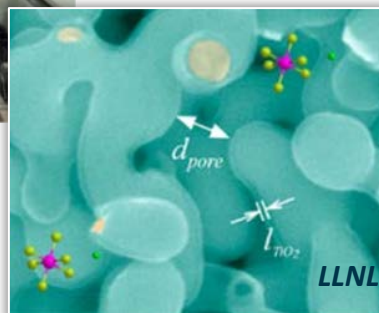


LAMMPS classic molecular dynamics modeling relevant to  $H_2O$  splitting

### Advanced Materials Synthesis

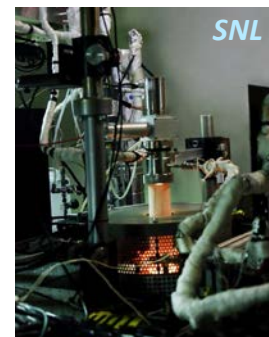


High-throughput spray pyrolysis system for electrode fabrication

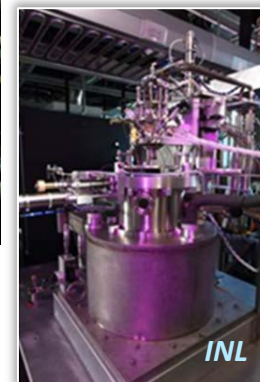


Conformal ultrathin  $TiO_2$  ALD coating on bulk nanoporous gold

### 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/>



# Approach/Accomplishments: Annual Review of Current and New Capability Nodes

Evaluated 5 new and >80 current capability nodes using the following 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
    - AWSM node utilization
    - Potential use by HydroGEN Seedling projects in the next project phase
    - Minor vs. major modifications

## 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

*Capability review is a rigorous process and keeps nodes updated and relevant*





# Accomplishments: Updated 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





# Accomplishments: Updated HydroGEN Website

Visit the HydroGEN website at <https://www.h2awasm.org>



Home About Capabilities Data **Publications** News Contact

## meeting the challenge

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

[Learn More](#)

### FEATURED CAPABILITY

[Techno-Economic Analysis of Hydrogen Production](#)

### IN THE NEWS

[Apply by April 9: Collaborative Interagency Opportunity for NSF DMREF...](#)

HydroGEN is a consortium of six U.S. Department of Energy (DOE) national laboratories that will address advanced water splitting materials challenges by making unique, world-class national lab capabilities in photoelectrochemical, solar thermochemical, and low- and high-temperature electrolytic water splitting more accessible to academia, industry, and other national labs. HydroGEN is part of the DOE Energy Materials Network (EMN) and is funded by DOE's Fuel Cell Technologies Office.

**4,632 users;**  
**24,452 pageviews;**  
**1,348 downloads**

**14**  
**news**  
**items**

**13**  
**journal**  
**articles**

**21**  
**presentations**



# Accomplishments: Publications and Patent Disclosures/Applications

*EMN is producing high-value R&D & disseminating it to the R&D community*

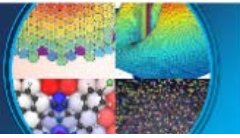
**nature energy** ARTICLES  
PUBLISHED: 31 JULY 2017 | VOLUME: 2 | ARTICLE NUMBER: 17127



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

Yuanyue Liu<sup>1,2</sup>, Jingjie Wu<sup>3</sup>, Ken P. Hackenberg<sup>3</sup>, Jing Zhang<sup>1</sup>, Y. Morris Wang<sup>2</sup>, Yingchao Yang<sup>1</sup>, Kuntal Keyshar<sup>1</sup>, Jing Gu<sup>3</sup>, Tadashi Ogitsu<sup>2</sup>, Robert Vajtai<sup>1</sup>, Jun Lou<sup>1</sup>, Pulickel M. Ajayan<sup>1</sup>, Brandon C. Wood<sup>2\*</sup> and Boris I. Yakobson<sup>1\*</sup>

**AIP** The Journal of Chemical Physics  
**PERSPECTIVES**

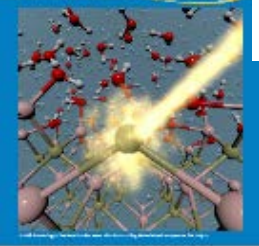


THE JOURNAL OF CHEMICAL PHYSICS 148, 071101 (2018)

**Communication: The electronic entropy of charged defect formation and its impact on thermochemical redox cycles**

Stephan Lary  
National Renewable Energy Laboratory, Golden, Colorado 80401, USA  
(Received 11 January 2018; accepted 6 February 2018; published online 16 February 2018)

The Journal of **PHYSICAL CHEMISTRY Letters**



**Integrating Ab Initio Simulations and X-ray Photoelectron Spectroscopy: Toward A Realistic Description of Oxidized Solid/Liquid Interfaces**

Tuan Anh Pham,<sup>1,2,3</sup> Xueqiang Zhang,<sup>4,5,6,7</sup> Brandon C. Wood,<sup>4,5</sup> David Prendergast,<sup>1,4</sup> Sylvia Ptasinska,<sup>4,5,6</sup> and Tadashi Ogitsu<sup>4,7</sup>

**J. Phys. Chem. Lett. 2018, 9, 194-203.**

**nature COMMUNICATIONS**



ARTICLE  
DOI: 10.1038/s41467-018-04067-9 OPEN

**A photochemical diode artificial photosynthesis system for unassisted high efficiency overall pure water splitting**

Faouzi A. Chowdhury<sup>1</sup>, Michel L. Trudeau<sup>2</sup>, Hong Guo<sup>3</sup> & Zetian Mi<sup>1,4</sup>

Fluid Phase Equilibria 460 (2018) 175–188

Contents lists available at ScienceDirect

**Fluid Phase Equilibria**

journal homepage: [www.elsevier.com/locate/fluid](http://www.elsevier.com/locate/fluid)

**Thermodynamic modeling of the hybrid sulfur (HyS) cycle for hydrogen production**

Harnoor Kaur<sup>a</sup>, Meng Wang<sup>a</sup>, Maximilian B. Gorenske<sup>b</sup>, Chau-Chyun Chen<sup>a,\*</sup>

<sup>a</sup> Department of Chemical Engineering, Texas Tech University, Lubbock, TX 79409-3121, USA  
<sup>b</sup> Savannah River National Laboratory, Aiken, SC 29802, USA



## Records of Invention (ROI) :

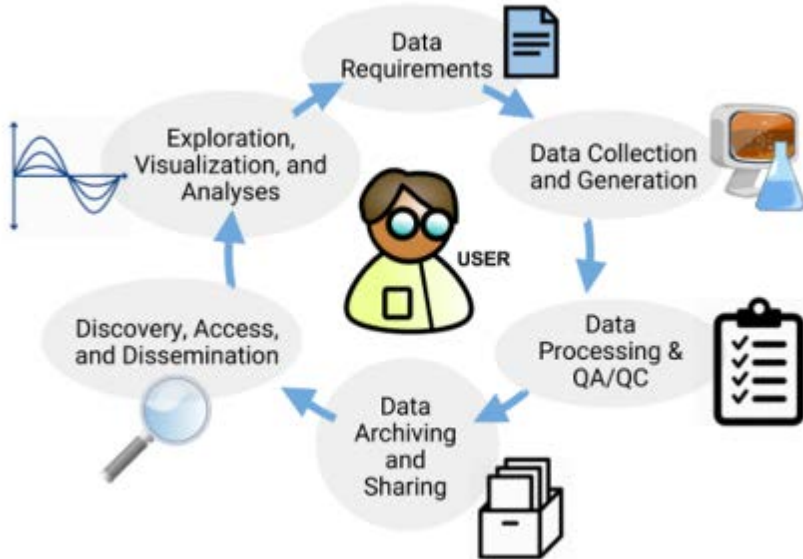
1. "High temperature solar reactor receiver for sulfuric acid decomposition," Z. Ma, J. Martinek, C. Corgnale, ROI-18-62 (2018).
2. "A novel electrochemical stack design for electrolysis or fuel cells," Z. Ma, ROI-18-65 (2018).



# Accomplishments/Data Management Plan: *HydroGEN Data Hub: Making digital data accessible*

## A Researcher Centric Approach

The HydroGEN Data Hub currently has  
135 users, >250 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





# Accomplishments: 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

- Developed and finalized a catalog of pre-approved, mutual agreements
  - ✓ Finalized and signed all **four** standard TT/A between all consortium partners
- Facilitated rapid IP, NDA, and contract agreements
  - ✓ **Executed all 19 project NDAs**





# Collaboration: 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, DOE-EERE-FCTO**



# Collaboration: NEW HydroGEN Seedling Projects

**19 proposals selected**, negotiated, and awarded (#proposals)

**44 unique capabilities** being utilized across six core labs

**Advanced Electrolysis (8)**

**LTE (5)**

**HTE (3)**

**PEC (5)**

**Benchmarking &  
Protocols (1)**

**STCH (5)**

**2-Step MO<sub>x</sub> (4)**

**Hybrid cycle (1)**





# National Innovation Ecosystem

## Collaboration/Accomplishments:

>100 samples exchanged

182 collaborators on the SharePoint site

4 collaborative white papers with NSF DMREF

26 papers published or submitted

2 Records of Inventions

Established AWSM literature database

User facility proposal submitted and personnel exchanged

EMN-wide Meeting on Machine Learning & Data Analytics



*HydroGEN kicked off a nationwide R&D effort (Nov. 2017), is vastly collaborative, and has produced many high value products*



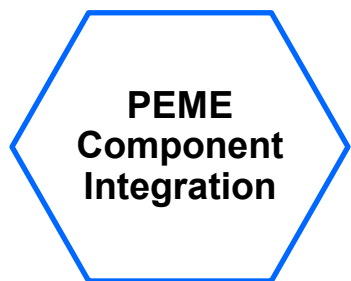


# A Balanced AWSM R&D Portfolio

## Accomplishments/Collaborations:



### Low Temperature Electrolysis (LTE) (G. Bender: PD148A; 5 Projects)



**PEM Electrolysis**

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

**AEM Electrolysis**

### High Temperature Electrolysis (HTE) (R. Boardman: PD148B; 3 Projects)

Degradation mechanism at high current density operation

**O<sup>2-</sup> conducting SOEC**

- Electrolyte and electrodes
- Low cost electrolyte deposition

**H<sup>+</sup> conducting SOEC**

### Photoelectrochemical (PEC) (A. Weber: PD148C; 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: PD148D; 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**



# Accomplishments: HydroGEN Benchmarking Advanced Water Splitting Technologies Project (PD170)

## 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

- Develop standardized best practices for characterizing and benchmarking AWSMs
- Foundation for accelerated materials RD&D for broader AWS community

## Accomplishments:

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

*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***



# Proposed Future Work

- Core labs will align scope of work with the relevant seedling projects' go/no-go decision points
  - Core labs' interaction with a specific seedling project will end if that project does not achieve its go/no-go decision metric
- 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 capabilities 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



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

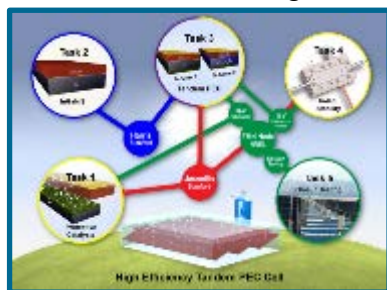
## Core Labs



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

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

Stanford University  
PEC Seeding



CU Boulder  
STCH Seeding



## A Nationwide Effort in Early-Stage R&D



HydroGEN  
Advanced Water Splitting Materials

### Meeting the Challenge

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



**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



**HydroGEN**  
Advanced Water Splitting Materials

This work was fully supported by the U.S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy (EERE), Fuel Cell Technologies Office (FCTO).



**Katie Randolph**



**David Peterson**



**James Vickers**



**Eric Miller**

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



# Acknowledgements



Energy Materials Network  
U.S. Department of Energy



**HydroGEN**  
Advanced Water Splitting Materials

## NREL Team

**Huyen Dinh, Lead  
Principal Investigators:**

Shaun Alia	Zhiwen Ma
Mowafak Al-Jassim	Kristin Munch
Guido Bender	Judy Netter
Jeff Blackburn	John Perkins
Kai Zhu	Bryan Pivovar
Todd Deutsch	Matthew Reese
Daniel Friedman	Genevieve Saur
David Ginley	Glenn Teeter
Kevin Harrison	Michael Ulsh
Steven Harvey	Judith Vidal
Stephan Lany	Andriy Zakutayev

## LBLN Team

**Adam Weber, Lead  
Principal Investigators:**

Nemanja Danilovic	Francesca Toma
Ian Sharp	Miquel Salmeron
Peter Agbo	Ethan Crumlin
David Larson	Jeffrey Greenblat
Lin-Wang Wang	Ahmet Kusoglu
Walter Drisdell	Frances Houle
Mike Tucker	David Prendergast

## SRNL Team

**Hector Colón-Mercado, Lead  
Principal Investigators:**

Maximilian Gorensek    Brenda Garcia-Diaz

# Acknowledgements



Energy Materials Network  
U.S. Department of Energy



**HydroGEN**  
Advanced Water Splitting Materials

## SNL Team

**Anthony McDaniel, Lead  
Principal Investigators:**

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

## LLNL Team

**Tadashi Ogitsu, Lead  
Principal Investigators:**

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

## INL Team

**Richard Boardman, Lead  
Principal Investigators:**

James O'Brien	Ting He
Dong Ding	Gabriel Ilevbare
Rebecca Fushimi	Soe Lwin
Dan Ginosar	Carl Stoots



# Technical Backup Slides





# 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	<b>Complete Nov. 2017</b>
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	<b>Complete</b>
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	<b>On Track</b>
Benchmark solar-to-hydrogen efficiency of best-in-class LiCoO <sub>2</sub> anode and Ni <sub>5</sub> P <sub>4</sub> cathode catalysts integrated on an upright GaInP <sub>2</sub> /GaAs tandem cell with a target of greater than 10%.	9/30/2018	QPM	<b>On Track</b>



# Collaborations: HydroGEN Expert Teams

Lab	Technical Experts	Data Experts	Technology Transfer Agreement (TT/A) Experts
NREL	Huyen Dinh	Kristin Munch, Robert White	Jean Schulte (MTA), Eric Payne (IPMP), Megan Ballweber (NDA) Anne Miller (CRADA)
SNL	Anthony McDaniel	Richard Karnesky	Rachel Wallace (IPMP, MTA, NDA) Jason Martinez (CRADA)
LBNL	Adam Weber	Dan Gunter	Catherine Koh (MTA, NDA), Betsy Quayle (CRADA), Shanshan Li (IPMP)
INL	Richard Boardman	Shyam Nair Robert Kinoshita	Ryan Bills (IPMP, NDA) Tara L. Justesen (CRADA, MTA)
LLNL	Tadashi Ogitsu	Thomas Yong-Jin (Yong) Han	Annemarie Meike
SRNL	Hector Colon-Mercado	Hector Colon-Mercado	Scott McWhorter