



Energy Materials Network  
U.S. Department of Energy



**HydroGEN**  
Advanced Water Splitting Materials



U.S. DEPARTMENT OF  
**ENERGY**

Energy Efficiency &  
Renewable Energy

# An Overview of HydroGEN: A DOE Energy Materials Network, Aimed at Accelerating the R&D of Advanced Water Splitting Materials (AWSM)

H.N. Dinh, E.L. Miller, K. Randolph, A. Weber, A. McDaniel,  
R. Boardman, T. Ogitsu, and H. Colon-Mercado

Date: 11/8/2017

Venue: Fuel Cell Seminar, Long Beach, CA

Renewable Hydrogen Pathways Session

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





# Energy Materials Network (EMN)



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U.S. Department of Energy



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The Energy Materials Network (EMN) aims to dramatically decrease time-to-market for advanced materials that are critical to many clean energy technologies.

### WORLD-CLASS INNOVATION

EMN is fueling U.S. industry with leading scientific and technical capabilities, data, and tools, and helping deliver innovative clean energy products to the world marketplace through its network of national lab-led consortia.

### CLEAR POINTS OF ENGAGEMENT

In building an enduring, accessible network, EMN offers industry clear points of engagement and streamlined access to national lab resources by providing technical support, collaboration tools, and data platforms.

### RAPID SCALE-UP

EMN is addressing market deployment barriers and getting new technologies to market faster by better integrating all phases of the materials development cycle, from discovery through deployment.



PROPELLING CLEAN ENERGY MATERIALS DEVELOPMENT FORWARD,  
2X FASTER AND AT HALF THE COST

EMN's initial consortia are focusing on targeted materials tracks aligned with some of industry's most pressing clean energy materials challenges.

LIGHTWEIGHT MATERIALS  
FOR VEHICLES

DURABLE MATERIALS FOR  
SOLAR MODULES

CALORIC MATERIALS FOR  
HEAT PUMP TECHNOLOGIES








NEXT-GENERATION ELECTRO-  
CATALYSTS FOR FUEL CELLS



# Current EMN Consortia Overview



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U.S. Department of Energy

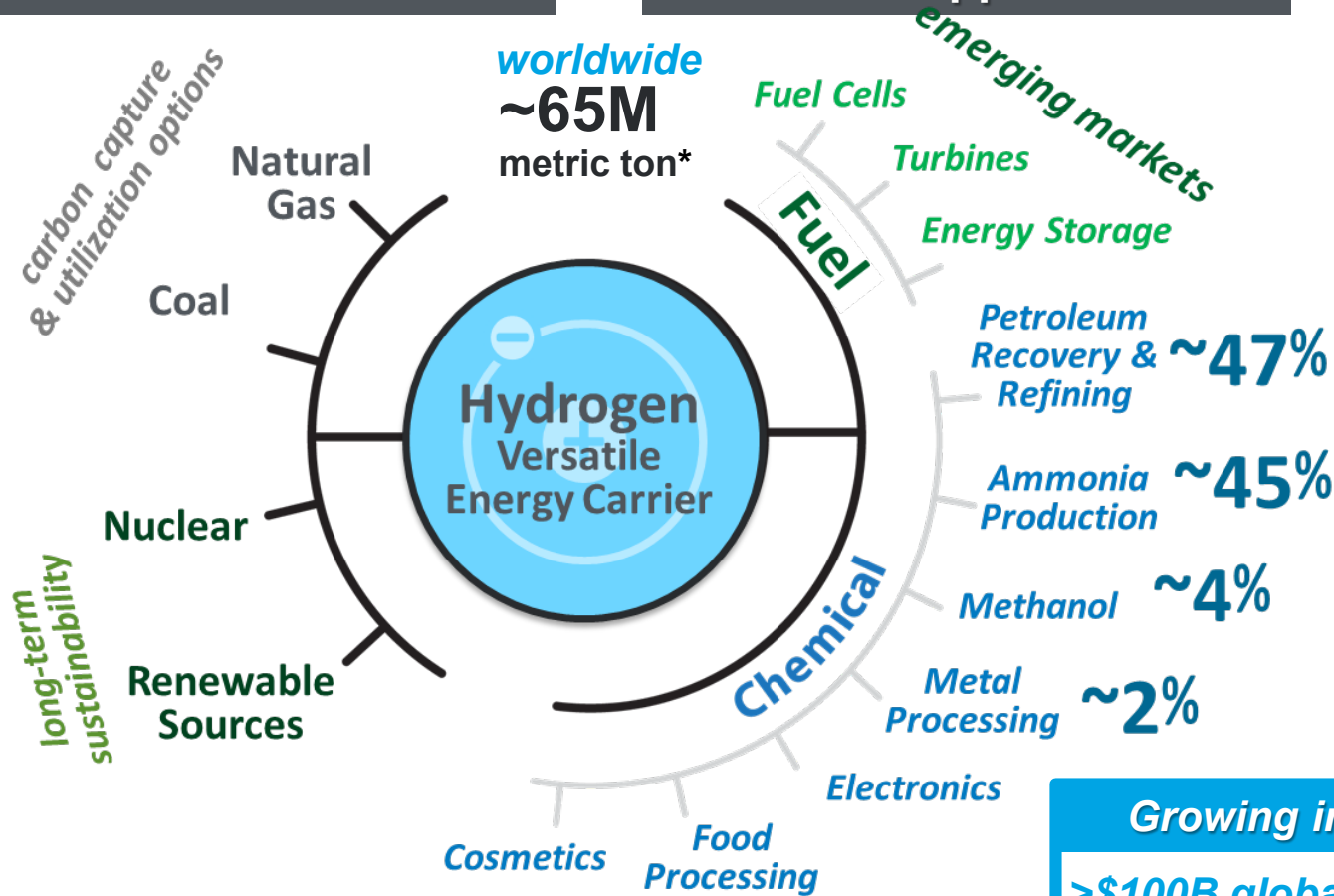
	<p>Caloric materials for efficient cooling and heat pumping technologies.</p>
	<p>Catalytic materials for commercial bioenergy applications</p>
	<p>Durable module materials that reduce the levelized cost of energy of photovoltaic systems.</p>
	<p>Lightweight materials for automotive manufacturing.</p>
	<p>Platinum group metal-free catalysts for automotive fuel cells</p>
	<p>Hydrogen storage materials by providing capabilities and foundational understanding.</p>
	<p>Advanced water splitting technologies for clean, sustainable hydrogen production.</p>



# Goal: Widespread H<sub>2</sub> Production & Delivery

## Diverse Sources

## Diverse Applications



**Growing industrial demand for H<sub>2</sub>**  
**>\$100B global market and expanding**

**Hydrogen enables domestic energy & environmental security, with large-scale market potential & with job creation and economic growth opportunities**





# HydroGEN Consortium Launch

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



[About](#) [Capabilities](#) [FAQs](#) [News](#) [Contact](#)

## meeting the challenge

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

[Learn More](#)

### FEATURED CAPABILITY

[Photoelectrochemical Device In Situ and Operando Testing Using X-Rays](#)

### IN THE NEWS

[Energy Department Announces \\$30 Million Investment for Innovation in...](#)

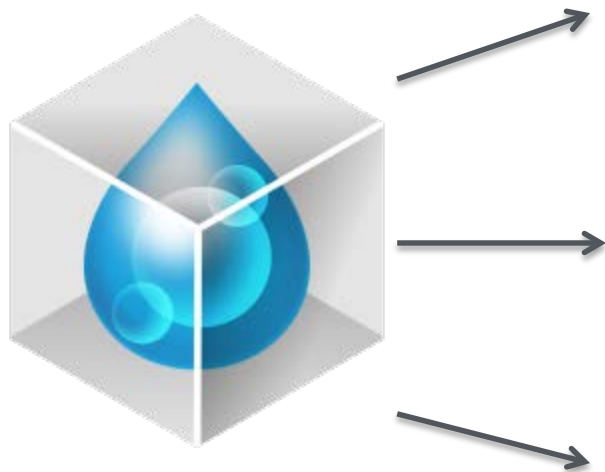
*Visit the HydroGEN website at <https://www.h2awsm.org>*



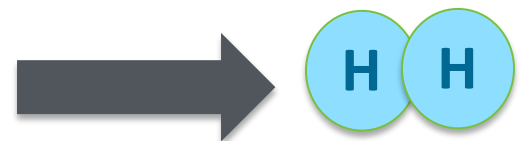
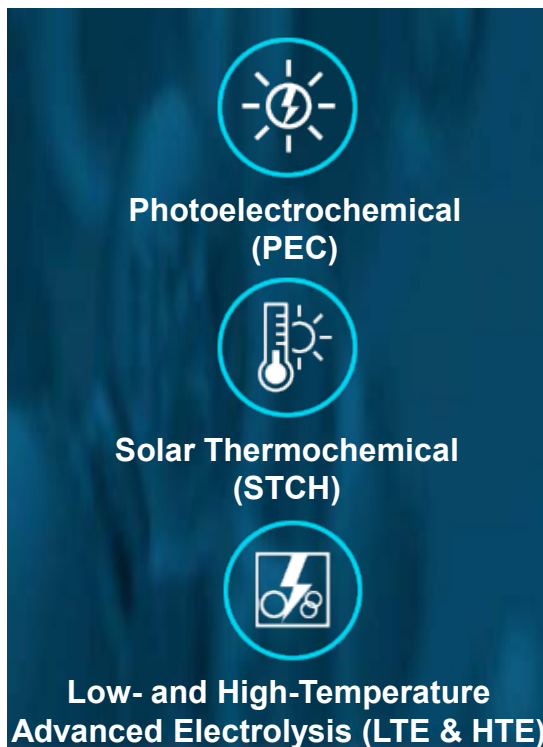
# HydroGEN: Advanced Water-Splitting Materials (AWSM) Consortium



**Accelerating discovery & development of innovative materials critical to advanced water splitting technologies for sustainable H<sub>2</sub> production, including:**



**Water**



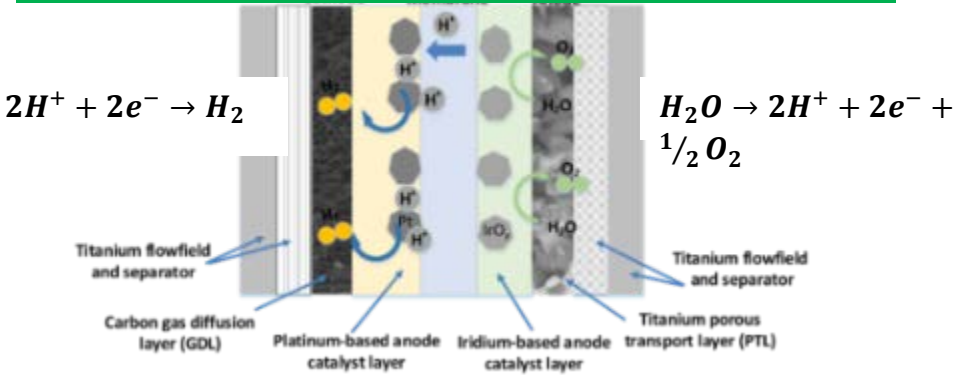
**Hydrogen**

**Website:  
[www.h2aws.org/](http://www.h2aws.org/)**

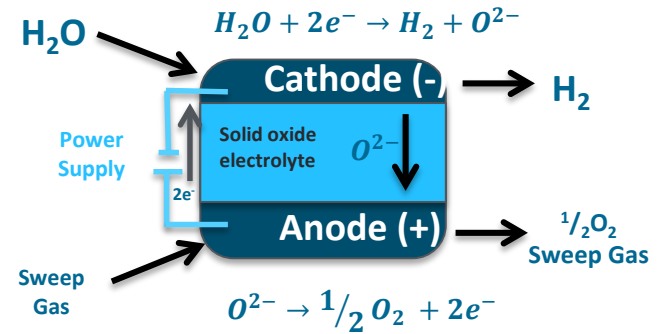


# Cross-Cutting Multiple Advanced Water Splitting Material (AWSM) Technologies

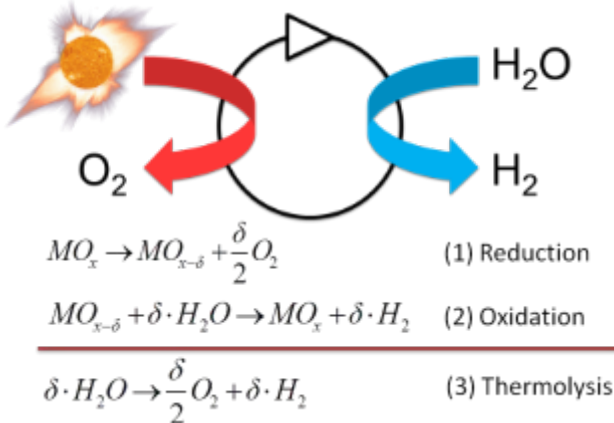
## Polymer Electrolyte Membrane Electrolysis (LTE)



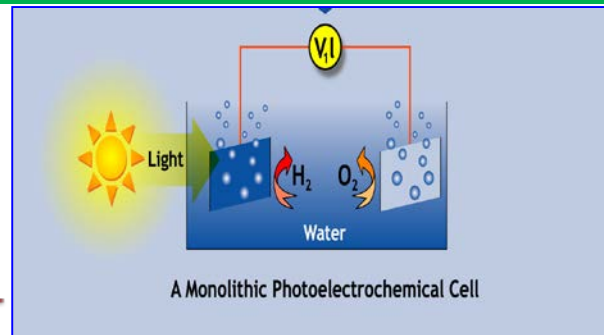
## Solid Oxide Electrolysis (HTE)



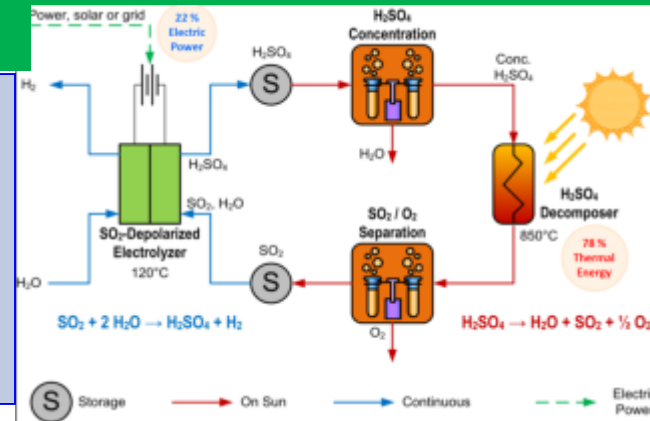
## Solar Thermochemical (STCH)



## Photoelectrochemical (PEC)



## Hybrid Sulfur Cycle (HT)

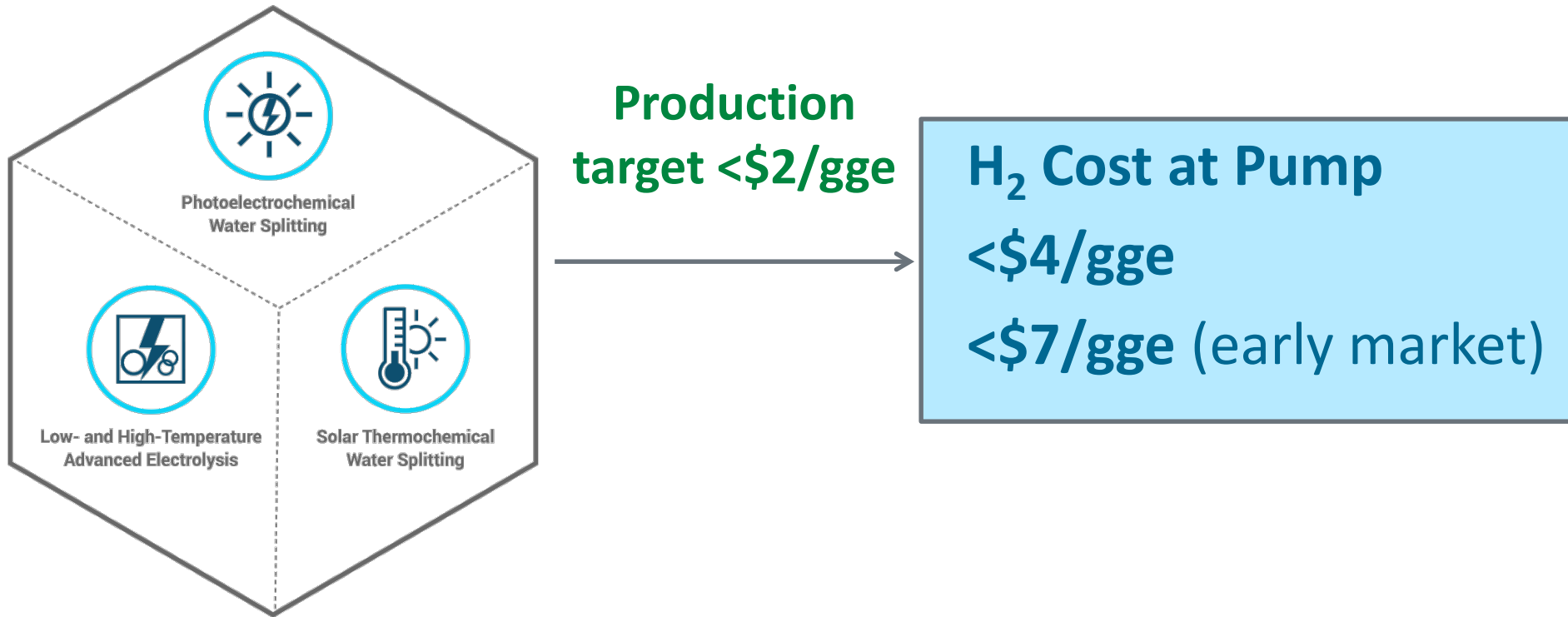


Hybrid = Electrolysis + STCH



# Cross-Cutting Technologies and Collaboration Can Enable Reduction in H<sub>2</sub> Production Cost

**RD&D from different water splitting pathways is critical to reducing renewable H<sub>2</sub> production cost**







# Collaborations: 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**

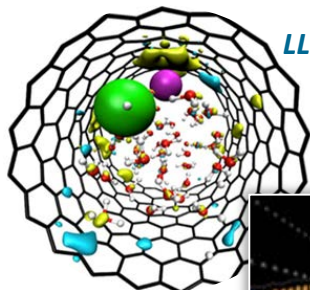




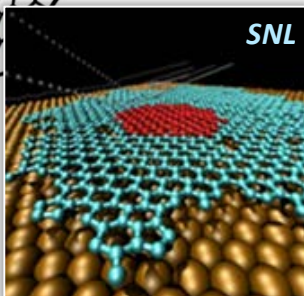
# HydroGEN: Advanced Water-Splitting Materials (AWSM) Consortium

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

## Materials Theory/Computation

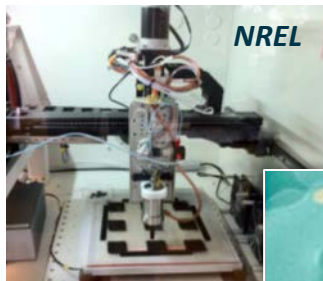


Bulk & interfacial models of aqueous electrolytes

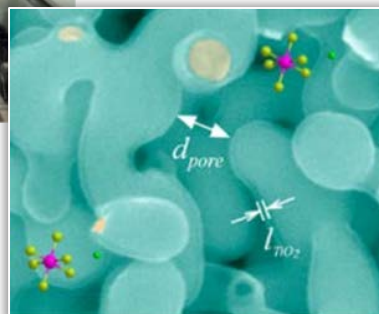


LAMMPS classic molecular dynamics modeling relevant to  $H_2O$  splitting

## Advanced Materials Synthesis

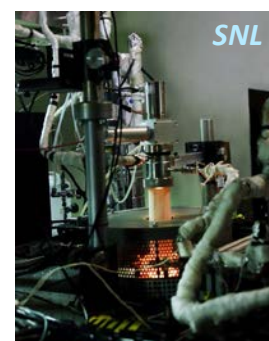


High-throughput spray pyrolysis system for electrode fabrication

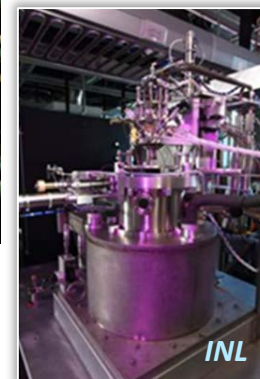


Conformal ultrathin  $TiO_2$  ALD coating on bulk nanoporous gold

## Characterization & Analytics



Stagnation flow reactor to evaluate kinetics of redox material at high-T



TAP reactor for extracting quantitative kinetic data

**Cross technology collaboration opportunities**

Website: <https://www.h2aws.org/>



# HydroGEN Website – Enhanced Capability Search

## LIST OF CAPABILITIES

Showing 1 to 12 of 82 entries

1 2 3 4 Next

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

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



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## 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 Home Page**  
(<https://datahub.h2awsm.org/>)

HydroGEN: Advanced Water Splitting Materials







# Technology Transfer Activities

## Non-Disclosure Agreement (NDA)

Information Disclosure

## Intellectual Property Management Plan (IPMP)

IP Protection

## ➤ Streamlined Access

## Materials Transfer Agreement (MTA)

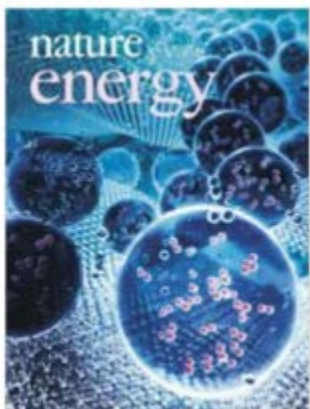
Freedom to Operate

## Cooperative Research and Development Agreement (CRADA)

Collaboration (nearly complete)

- Developed a catalog of pre-approved, mutual agreements between all consortium partners
- Facilitating rapid IP, NDA, and contract agreements





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

Yuanyue Liu<sup>1†‡</sup>, Jingjie Wu<sup>1‡</sup>, Ken P. Hackenberg<sup>1‡</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>



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



# High Impact Publications & Patents

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



## Mass-spectrometer based Faradaic efficiency system



## Protected Layer to Enhance Durability



- Filed provisional patent on “PASSIVATING WINDOW AND CAPPING LAYER FOR PHOTOELECTROCHEMICAL CELLS.” on August 16, 2016 at the United States Patent & Trademark Office (USPTO) and has received Application No. 62/375,718.
- Filed a non-provisional patent on “Devices and Methods for Photoelectrochemical water splitting” March 23<sup>rd</sup>, 2016 based on our IMM for high efficiency work. United States Patent Application 20160281247. Awaiting examination.

**High Impact Publications and Patent Applications**





# NEW HydroGEN Seedling Project

**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<sub>x</sub> (4)**  
**Hybrid cycle (1)**



*To learn more, check HydroGEN website or contact [huyen.dinh@nrel.gov](mailto:huyen.dinh@nrel.gov)*





# HydroGEN EMN

Website:  
[www.h2awsm.org/](http://www.h2awsm.org/)

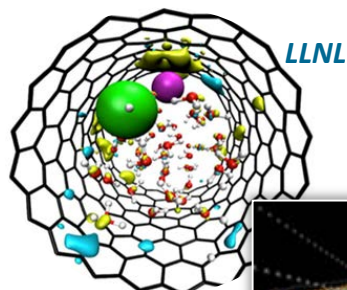


## Core Labs

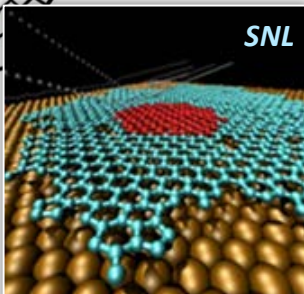


Comprising more than 80 unique, world-class capabilities/expertise in materials theory/computation, synthesis, and characterization & analysis:

### Materials Theory/Computation

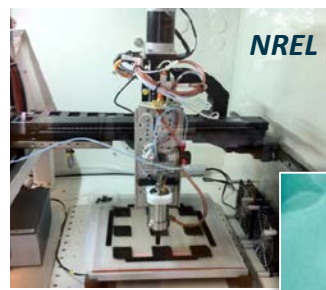


Bulk and interfacial models of aqueous electrolytes

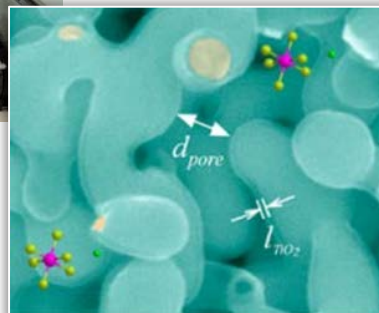


LAMMPS classic molecular dynamics modeling relevant to H<sub>2</sub>O splitting

### Advanced Materials Synthesis

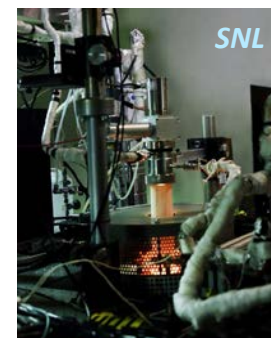


High-throughput spray pyrolysis system for electrode fabrication

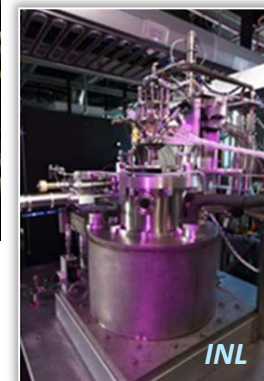


Conformal ultrathin TiO<sub>2</sub> ALD coating on bulk nanoporous gold

### Characterization & Analysis



Stagnation flow reactor to evaluate kinetics of redox material at high-T



TAP reactor for extracting quantitative kinetic data

**HydroGEN is enabling innovative, world-class research of water-splitting materials and catalysts.**

# Acknowledgements



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U.S. Department of Energy



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U.S. DEPARTMENT OF  
**ENERGY**

Energy Efficiency &  
Renewable Energy

## DOE EERE Fuel Cell Technology Office Team

**Eric Miller and  
Katie Randolph,  
(Leads)**

**David Peterson  
James Vickers  
Maxim Lyubovsky  
Kim Cierpik-Gold**



# Acknowledgements



Energy Materials Network  
U.S. Department of Energy



**HydroGEN**  
Advanced Water Splitting Materials

## NREL Team

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Jeff Blackburn	John Perkins
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Todd Deutsch	Matthew Reese
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Steven Harvey	Judith Vidal
Stephan Lany	Andriy Zakutayev

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Lin-Wang Wang	Ahmet Kusoglu
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Mike Tucker	David Prendergast

## SRNL Team

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

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# Acknowledgements



Energy Materials Network  
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**HydroGEN**  
Advanced Water Splitting Materials

## SNL Team

**Anthony McDaniel, Lead  
Principal Investigators:**

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Bert Debusschere	John Mitchell
Farid El Gabaly	Jeff Nelson
Lindsay Erickson	Peter Schultz
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Ethan Hecht	Alan Wright
Reese Jones	

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**Tadashi Ogitsu, Lead  
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Tae Wook Heo	Trevor Willey
Jonathan Lee	Brandon Wood
Miguel Morales-Silva	Marcus Worsley
Christine Orme	

## INL Team

**Richard Boardman, Lead  
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Dong Ding	Gabriel Ilevbare
Rebecca Fushimi	Soe Lwin
Dan Ginosar	Carl Stoots