



# HydroGEN: A Consortium on Advanced Water Splitting Materials

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T. Ogitsu, H. Colon-Mercado

Presenter: Huyen Dinh, NREL

Date: 6/8/2017

Venue: 2017 DOE Annual Merit Review

Project ID # PD148

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# HydroGEN Overview

## Timeline and Budget

- Start date (launch): **June 2016**
- Total DOE funds received to date: **\$3.6M**

## Barriers

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

## Partners





# Advanced Water Splitting Materials Workshop April 2016 Stanford

Assembled experts to identify cross-cutting research needs to accelerate materials discovery for sustainable H<sub>2</sub> production

Advanced Electrolysis

Low & High

Photoelectrochemical

Solar Thermochemical

Hybrid Thermochemical





# Major Outcomes from Stanford Workshop

- Detailed techno-economic (TEA) and greenhouse gas (GHG) emission analyses are important
- Accurate TEA requires a strong understanding of **full system** requirements
- Well-defined **materials metrics** connected to **device- and system-level metrics** are important
- **Cross technology collaboration opportunities**
  - Common materials challenges and opportunities exist between High-T electrolysis and STCH, including **active- and BOP-materials**
  - **Catalyst** discovery and development needs and opportunities are common to PEC and Low-T electrolysis
  - **Membranes/separations materials** research is needed for all technologies

Establish HydroGEN EMN consortium on  
Advanced Water Splitting Materials



# Relevance – Energy Materials Network (EMN)



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

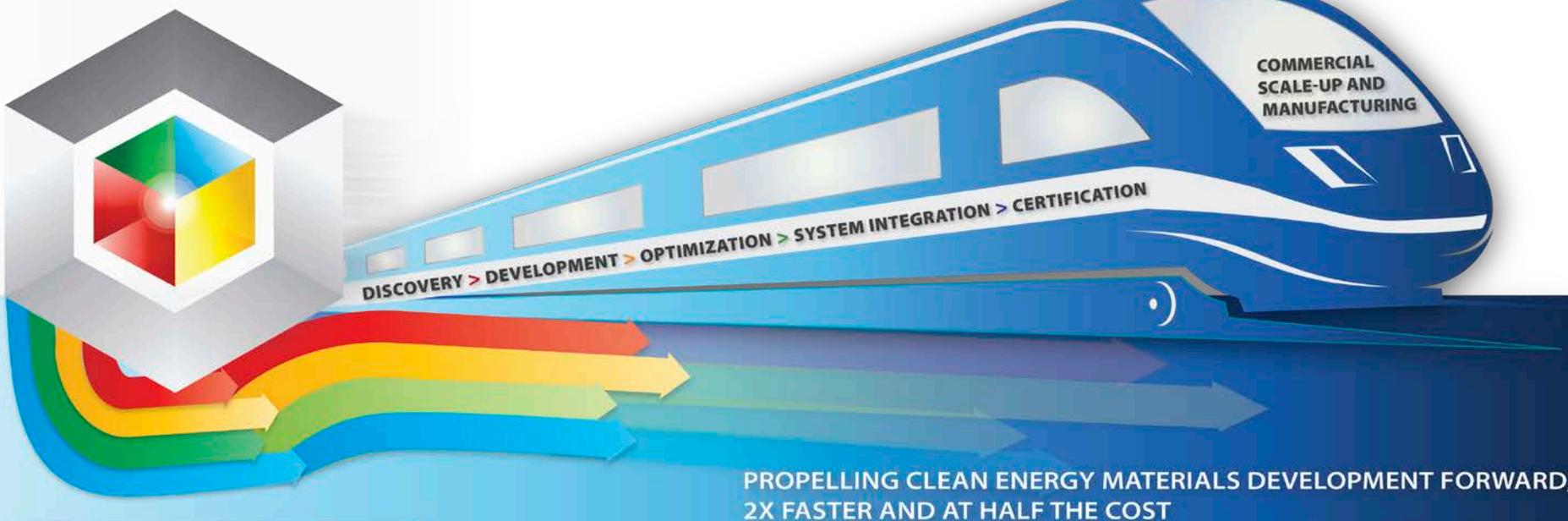
EMN is fueling U.S. industry with leading scientific and technical capabilities, data, and tools, and helping deliver innovative clean energy products to the world marketplace through its network of national lab-led consortia.

### 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.



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



# Relevance – Goals of EMN Consortia

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



# HydroGEN Energy Materials Network (EMN)

## Relevance, Overall Objective, and Impact

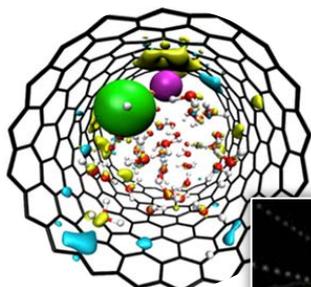


### Core Labs

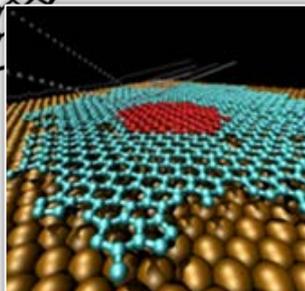


Comprising more than 80 unique, world-class capabilities/expertise in materials theory/computation, synthesis, and characterization & analysis:

#### Materials Theory/Computation

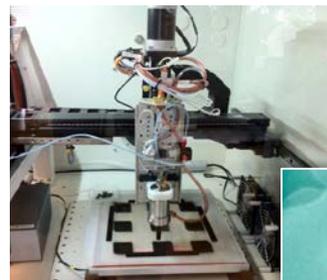


Bulk and interfacial models of aqueous electrolytes

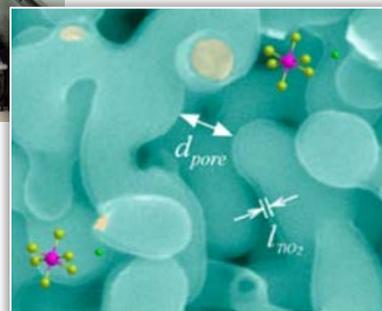


LAMMPS classic molecular dynamics modeling relevant to  $H_2O$  splitting

#### Advanced Materials Synthesis

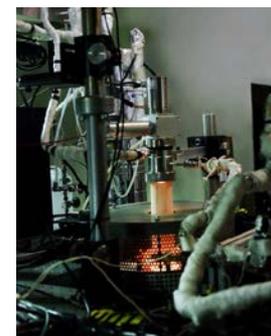


High-throughput spray pyrolysis system for electrode fabrication

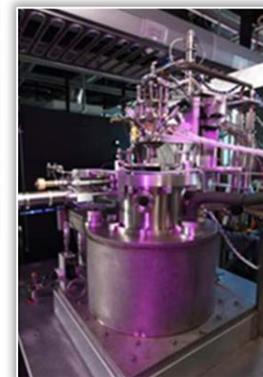


Conformal ultrathin  $TiO_2$  ALD coating on bulk nanoporous gold

#### Characterization & Analysis



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



TAP reactor for extracting quantitative kinetic data

**HydroGEN fosters cross-cutting innovation using theory-guided applied materials R&D to advance all emerging water-splitting pathways for hydrogen production**



# 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, DOE-EERE-FCTO**



# Collaborations: Established the HydroGEN Expert Teams

Lab	Technical Experts	Data Experts	Technology Transfer Agreement (TT/A) Experts
NREL	Huyen Dinh	Kristin Munch, Robert White	Doreen Molk (IPMP, 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	Carl Stoots	Ryan Bills (IPMP, NDA) Benjamin Louderback (CRADA, MTA)
LLNL	Tadashi Ogitsu	Thomas Yong-Jin (Yong) Han	Annemarie Meike
SRNL	Hector Colon- Mercado	Hector Colon- Mercado	Scott McWhorter

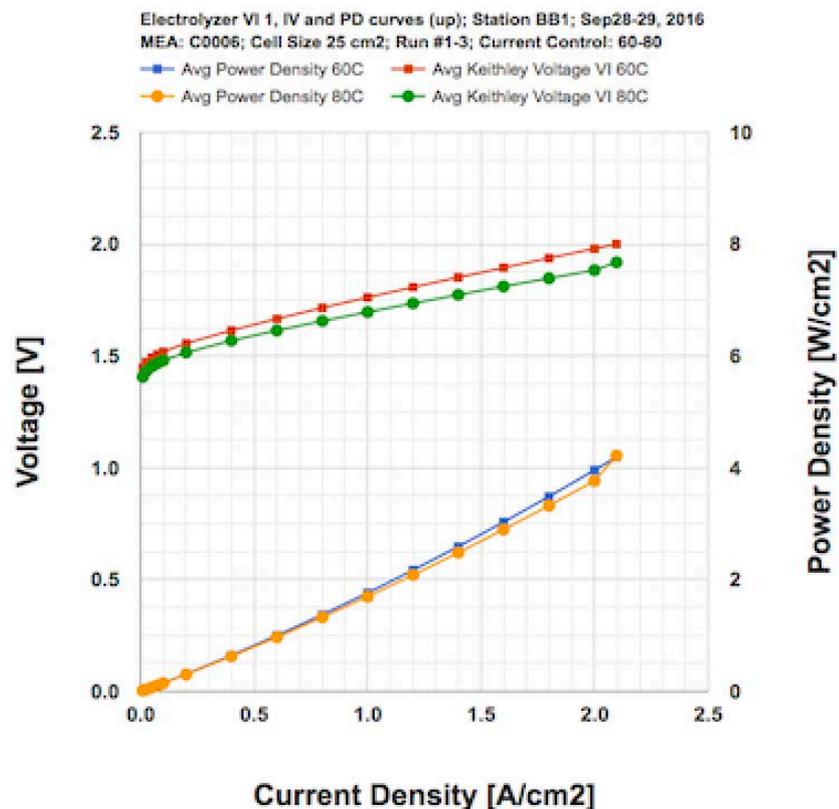
**Data Experts also meet biweekly via telecom/webcast**



# Accomplishments: HydroGEN Data Team Activities

## HydroGen DataHub LIVE

DataHub Plug-ins have been developed for electrolysis performance testing data



### Purpose of Data Team:

- Making digital data accessible

### Data Team Activities:

- Data Hub prototyping since Dec. 2016
  - Data Hub implemented in May 2017
- Leveraging other EMN's Data Teams for best practices & code sharing and authentication





# 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
- Finalized and signed 3 of 4 standard Technology Transfer and Agreements (TT/A)





# Accomplishments: Established HydroGEN Website

> 80 capabilities

1,382 users  
4,839 pageviews  
998 PDF downloads



**HydroGEN**  
Advanced Water Splitting Materials

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

Photoelectrochemical Water Splitting  
Solar Thermochemical Water Splitting  
Low- and High-Temperature Advanced Electrolysis

The HydroGEN Advanced Water Splitting Materials consortium aims to accelerate the research, development, and deployment of advanced water splitting technologies for clean, sustainable hydrogen production.

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.

Contact Us ›

Capabilities ›

FAQs ›

## HydroGEN Webinars

View recent webinars describing the capabilities in each of the three water splitting pathways covered by HydroGEN:

- Part 1: Photoelectrochemical (PEC) Water Splitting
- Part 2: Electrolysis
- Part 3: Solar Thermochemical (STCH) Hydrogen Production

Users clicked on the HydroGEN contact email (<mailto:h2awsm@nrel.gov>) 285 times.

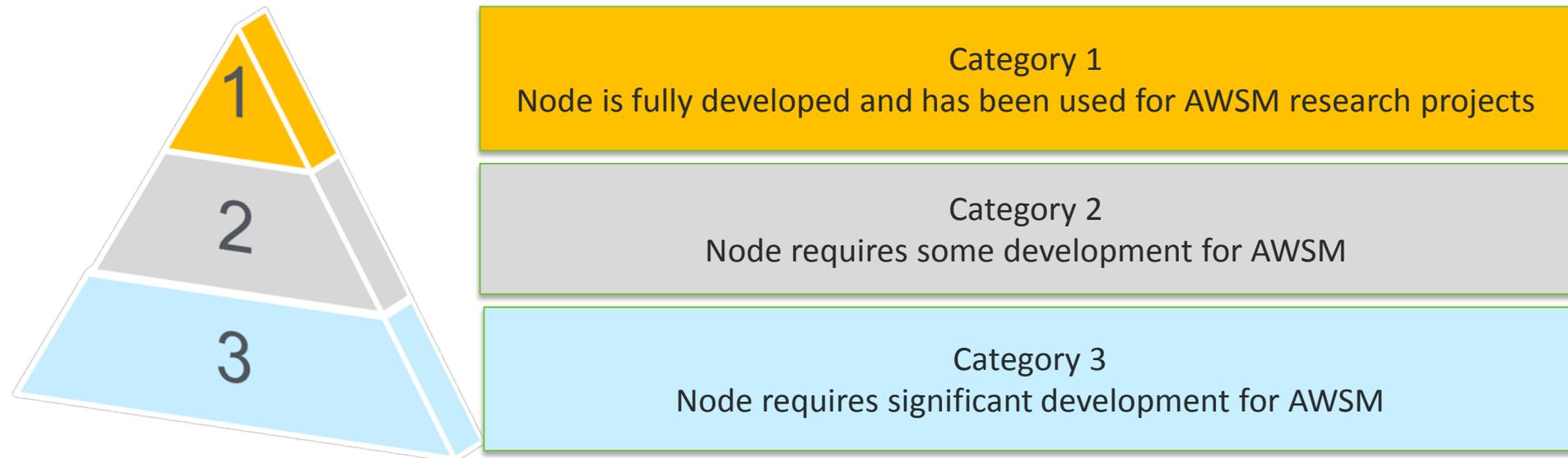


# Accomplishments: Established Capability Node Evaluation Criteria and Process

## 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



# Accomplishments: New HydroGEN Website – Enhanced Capability Search

## 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)

Show

Showing 1 to 12 of 82 entries

<p>Ab Initio Modeling of Electrochemical Interfaces</p> <p>LLNL      PEC 1, LTE 2</p>	<p>Advanced Electron Microscopy</p> <p>SNL      HTE 1, LTE 1, PEC 1, STCH 1</p>	<p>Advanced Materials for Water Electrolysis at Elevated Temperatures</p> <p>INL      HTE 2</p>
<p>Advanced Water-Splitting Materials Requirements Based on Flowsheet Development and Techno-Economic A...</p> <p>SRNL      HT 1, HTE 1, STCH 2, LTE 3, PEC 3</p>	<p>Albany: Open-Source Multiphysics Research Platform</p> <p>SNL      HTE 1, LTE 1, PEC 1, STCH 1</p>	<p>ALD Based Surface Functionalization and Porosity Control</p> <p>LLNL      PEC 3</p>
<p>Analysis and Characterization of Hydrided Material Performance</p> <p>INL      HTE 2</p>	<p>Beyond-DFT Simulation of Energetic Barriers and Photoexcited Dynamics</p> <p>LLNL      PEC 2</p>	<p>Cascading Pressure Reactor</p> <p>SNL      STCH 1</p>

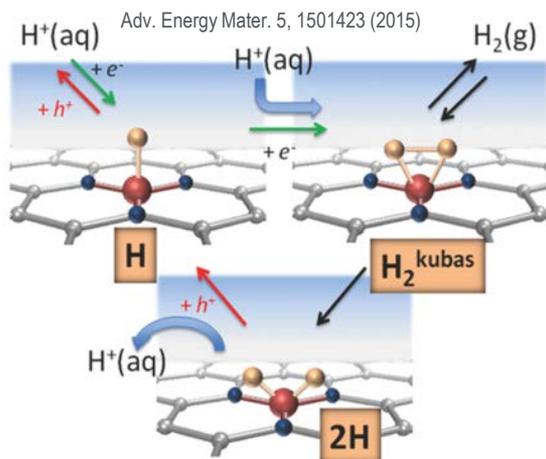




# Accomplishments: >80 Water Splitting Capability Nodes

Technology	Total	Category 1	Category 2	Category 3
AE	59	23	31	5
PEC	57	34	15	8
STCH	40	18	13	9

## Materials Theory/Computation



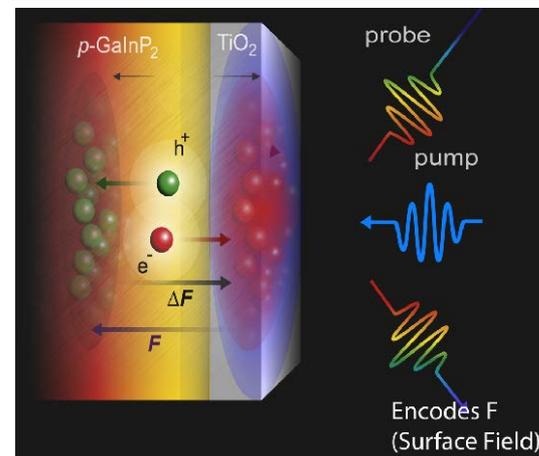
Catalytic activity predictions using *ab initio* descriptors

## Advanced Materials Synthesis



State-of-the-art ultrahigh vacuum (UHV) CIGS cluster tool

## Characterization & Analysis



Transient Photoreflectance for Electro-optical Characterization of Photoelectrochemical Materials and Interfaces

Several nodes span multiple classification areas (analysis, synthesis, characterization, etc.) and different technologies (AE, PEC, STCH)

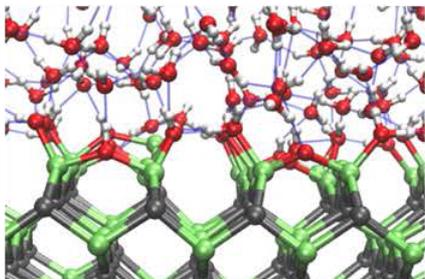


# Example Node: LLNL Ab-initio Modeling of Electrochemical Interfaces

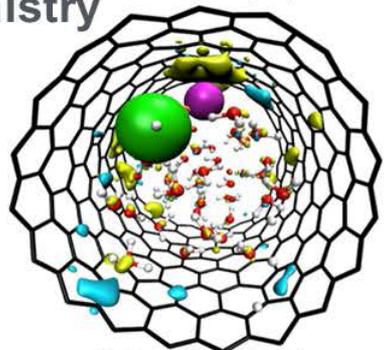
PEC : CAT 1

## Solid-liquid interfacial chemistry

JACS 135, 15774 (2013); Nat. Mater. (In press) JPCPC 120, 7332 (2016)



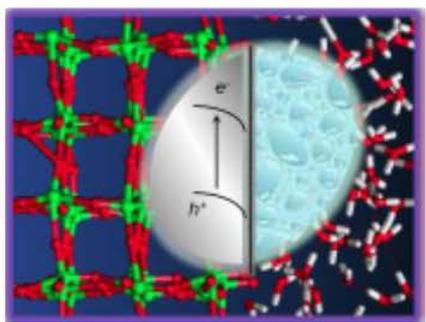
Ab initio molecular dynamics of semiconductor-water and metal-water interfaces



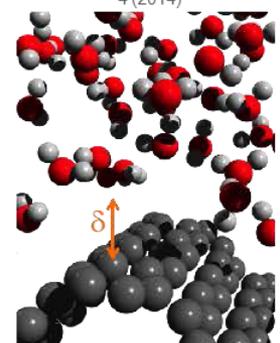
Bulk and interfacial properties of aqueous electrolytes

## Electronic properties of interfaces

JACS 136, 17071 (2014); PRB 89, 060202 (2014) PRB 91, 125415 (2015); JPCPC 118, 4 (2014)

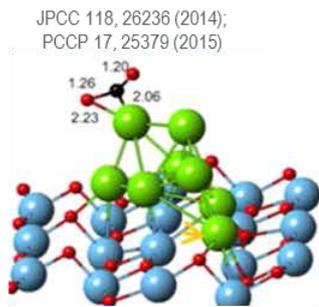
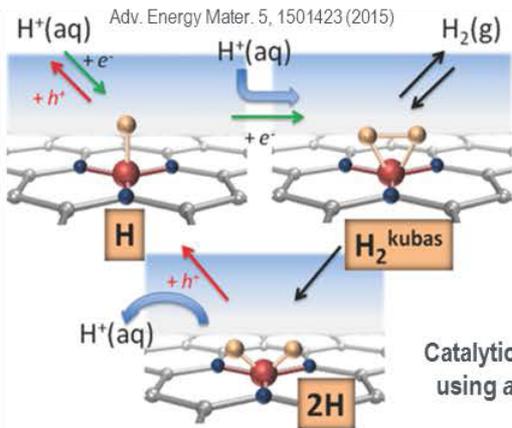


Electronic properties of electrode-electrolyte interfaces (from GW)



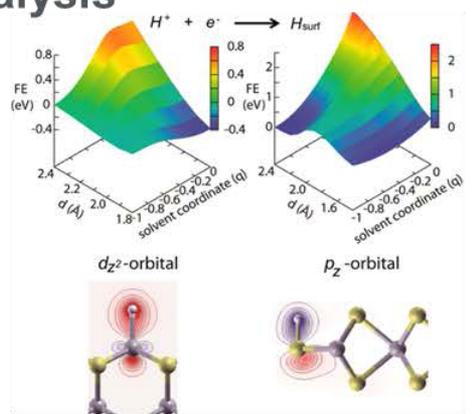
Simulations under applied bias or photobias

## Electrocatalysis and photocatalysis



Catalytic activity predictions using ab initio descriptors

Charge-transfer barriers for H<sub>2</sub> evolution



JPCPC 117, 21772 (2013)



# Example Node: NREL PEM Electrolyzer Testing Capabilities

LTE : CAT 1

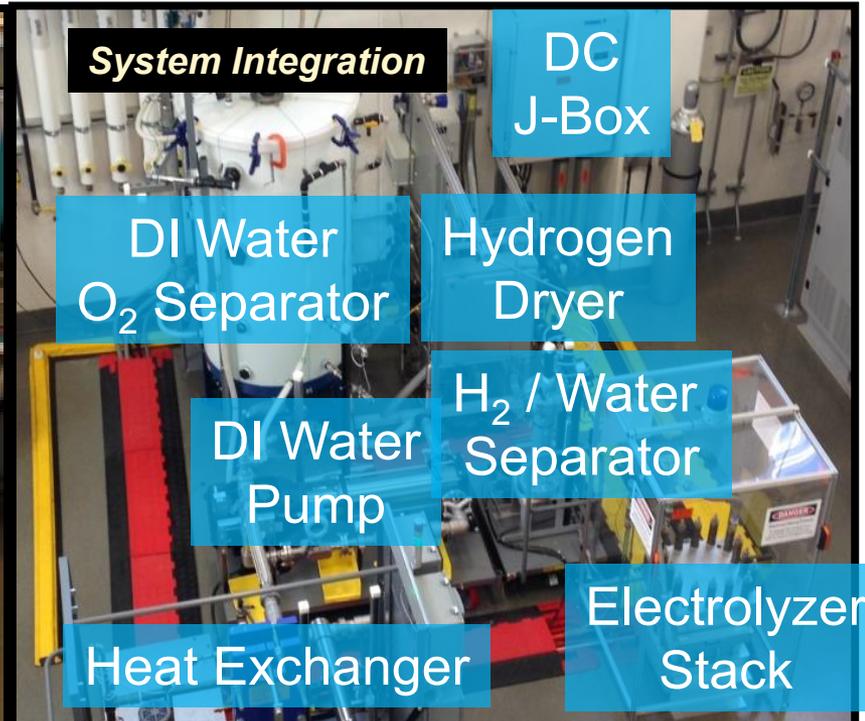
## Characterization & Analysis



### Greenlight Single Cell Test Systems

- 12V/250A power supply
- Up to 30 bar operation
- 5 cell voltage monitors
- AC impedance
- Anode and cathode product gas analyzer
- H<sub>2</sub> pump
- Up to 5 bar inlet pressure
- Up to 50 bar outlet pressure

## System Integration



DC  
J-Box

DI Water  
O<sub>2</sub> Separator

Hydrogen  
Dryer

DI Water  
Pump

H<sub>2</sub> / Water  
Separator

Heat Exchanger

Electrolyzer  
Stack

### Electrolyzer Stack Test Bed

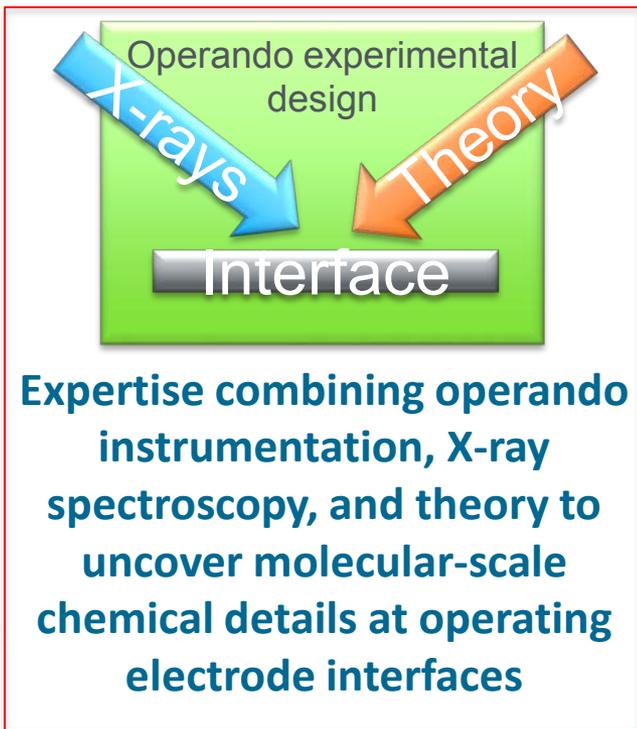
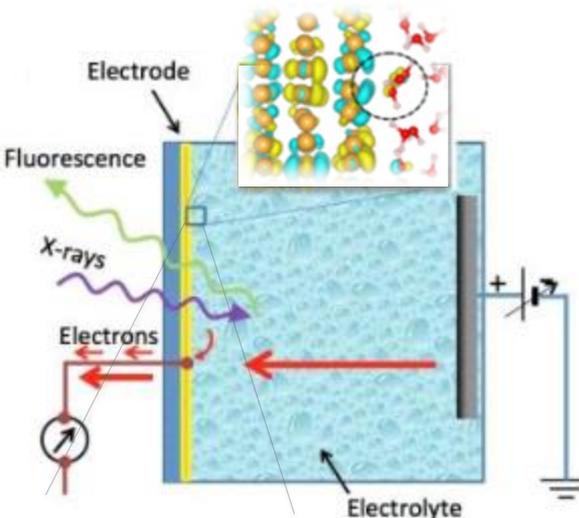
- Flexible platform
- Each system part exchangeable
- Large active area stack testing with 250 kW stacks demonstrated
- AC-DC power supplies (4,000 ADC and 250 VDC)



# Example Node: LBNL X-Ray Approaches for Understanding (Photo)Electrochemistry at Interfaces

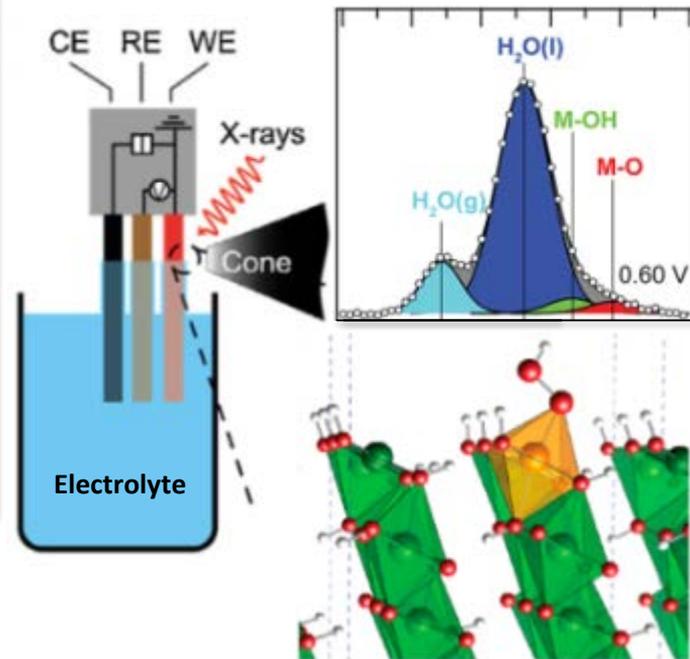
LTE, HTE : 1

## Operando XAS

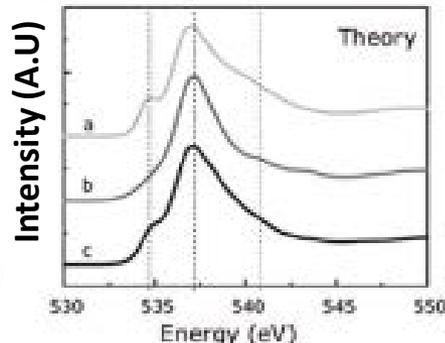
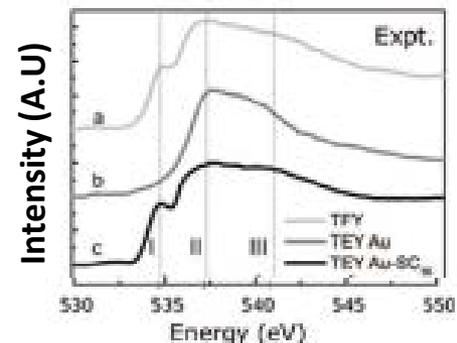


Expertise combining operando instrumentation, X-ray spectroscopy, and theory to uncover molecular-scale chemical details at operating electrode interfaces

## Operando ambient pressure XPS



X-ray photoelectron spectroscopy and molecular simulations reveal atomic concentration, chemical speciation, and potential profile at electrode interface



X-ray absorption spectroscopy, coupled to theory, reveals electronic and atomic structure of chemical species at electrode interface



# Example Node: SNL National Solar Thermal Test Facility (NSTTF)

STCH, HT : CAT 1



16 kW solar furnace

### Key Features:

- Operated by Sandia National Laboratories for the U.S. Department of Energy (DOE), the National Solar Thermal Test Facility (NSTTF) is the only test facility of this type in the United States.
- The NSTTF's primary goal is to provide experimental engineering data for the design, construction, and operation of unique components and systems in proposed solar thermal electrical plants planned for large-scale power generation.

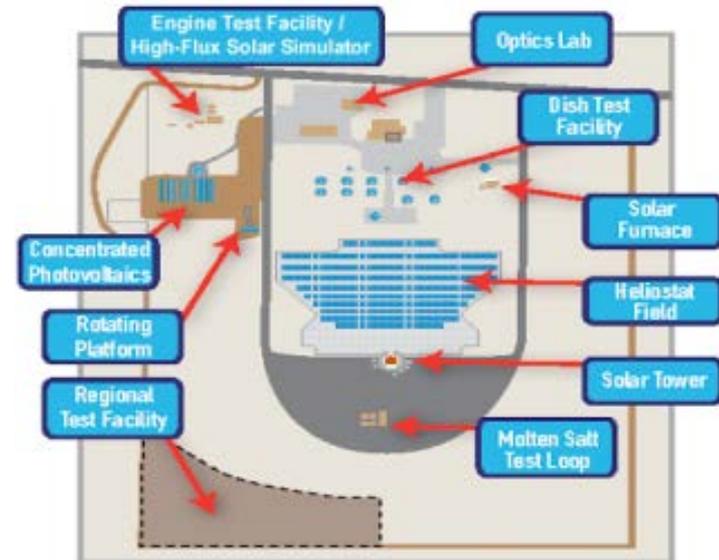
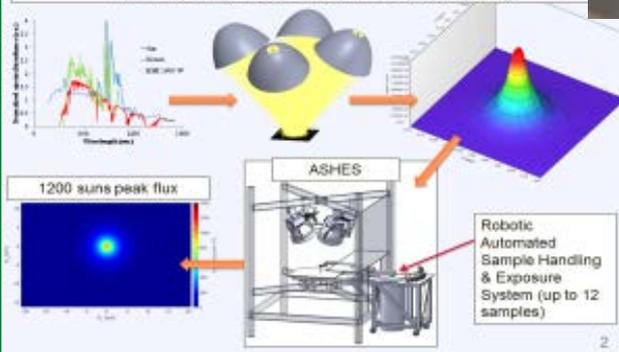
## High-flux solar simulator



6 MW power tower

### High-Flux Solar Simulator with Automated Sample Handling & Exposure System (ASHES)

Four 1.8 kW<sub>e</sub> metal-halide lamps produce up to 1200 suns



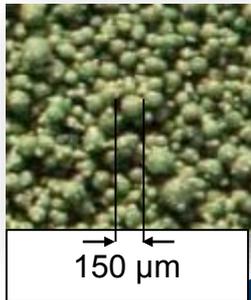
<http://energy.sandia.gov/energy/renewable-energy/solar-energy/csp-2/nsttf/>



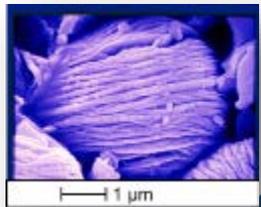
# Example Node: INL Commissioned 2<sup>nd</sup> TAP Reactor for Quantification of Catalyst Kinetics

HTE, STCH : CAT 2

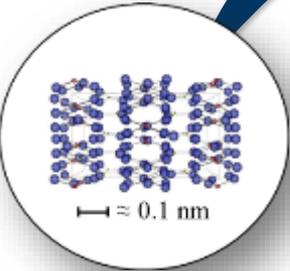
Spray dried catalyst form for attrition-resistant industrial use



SEM image of bulk catalyst particle with layered structure



(VO)<sub>2</sub>P<sub>2</sub>O<sub>7</sub> Crystal Structure



Molecular scale chemistry

Industrial process



Detailed chemical kinetics

Using complex materials, directly from an industrial operating environment

A unique top-down approach to material complexity

Elementary reaction steps, complex mechanism development

Industrial scale manufacture

Catalyst scale-up and forming processes

Temporal Analysis of Products (pulse response technique)  
Fundamental Kinetics of Industrial Catalysts Understood with TAP



INL now has two of three TAP Systems in the U.S.A.



# Example Node: SRNL High Temperature Materials Degradation & Corrosion Characterization and Mitigation for H<sub>2</sub> Production

HT, HTE : 3



- Electrochemical testing cells, immersion tests, and thermosiphon flow testing capabilities in walk-in hood
- Thermosiphon furnaces have three heating zones for temperature/flow velocity control
- Gas manifolds to ensure negligible or controlled introduction of impurities to cells
- Gloveboxes for handling of air/moisture sensitive materials



# Next Steps

- Integrate and support HydroGEN FOA-award winners
- Continue to maintain and develop HydroGEN capabilities nodes
- Identify new, relevant HydroGEN capability nodes
- Continue to develop a user-friendly and dynamic data portal that accelerates learning and information exchange among other EMN, AE, PEC, and STCH communities
- Continue to develop the HydroGEN data hub for research data repository, analysis tools, and secure data sharing within the HydroGEN EMN labs, with partners, and to the community
- R&D of HydroGEN critical materials
- Establish benchmarking and standard protocols and metrics for the different water splitting technologies
- Outreach
- Integrate whole system (capability nodes, FOA awardees, data infrastructure, TT/A) to accelerate materials development to deployment



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

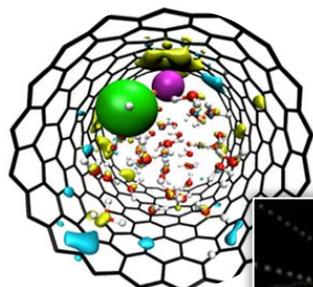


## Core Labs

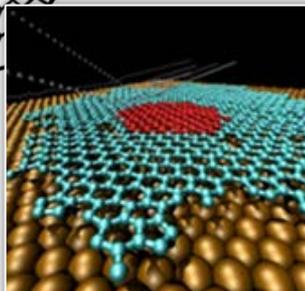


*Comprising more than 80 unique, world-class capabilities/expertise in materials theory/computation, synthesis, and characterization & analysis:*

### Materials Theory/Computation

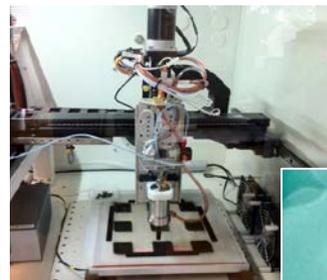


*Bulk and interfacial models of aqueous electrolytes*

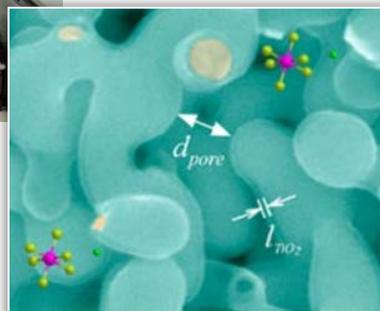


*LAMMPS classic molecular dynamics modeling relevant to H<sub>2</sub>O splitting*

### Advanced Materials Synthesis

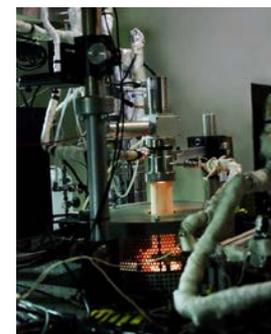


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*Conformal ultrathin TiO<sub>2</sub> ALD coating on bulk nanoporous gold*

### 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**

# 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

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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  
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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

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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



# Approach – FY2017 AOP Milestones

Milestone Name/Description	End Date	Type	Status
Launch HydroGEN consortium website including at least 50 distinct EMN capabilities nodes at 5 or more core national laboratories.	12/31/2016	Annual Milestone (Regular)	<b>Complete</b> <b>Oct. 2016</b>
Prepare and present in person to the US Drive Hydrogen Production Technology Team, providing an overview of the EMN model and the details of the HydroGEN Consortium objectives and available capabilities.	2/28/2017 <b>Modified to be due in April 2017 (Q3)</b>	QPM (Regular)	<b>Complete</b> <b>4/20/2017</b>
Publish library of standardized HydroGEN NDA and CRADA forms. <b>(3 of 4 TT/A have been completed)</b>	6/30/2017	QPM (Regular)	<b>On Track</b>
Launch online data portal and provide annual summary to DOE for the evaluation of HydroGEN, including effectiveness of nodes and utilization and lessons learned to share with other EMN consortia. Identify potential new EMN capabilities/nodes at 5 or more core national laboratories to be considered for support in FY18.	9/30/2017	QPM (Regular)	<b>On Track</b>



# Publications and Presentations

- “Hydrogen-induced Fermi-level pinning in chalcopyrite and kerterite absorbers from first-principles,” J. Varley, V. Lordi, T. Ogitsu, A. Deangelis, K. Horsley, and N. Gaillard, to be submitted.
- “Probing the Interplay between Chemistry and Electronic Properties of Native Oxides at Photoelectrchemical Interfaces,” T. A. Pham, X. Zhang, B. C. Wood, D. Prendergast, S. Ptasinska, and T. Ogitsu, under review.
- “Electrochemical hydrogen production,” T. He, P. Kar, N. McDaniel and B. Randolph, in *Springer Handbook of Electrochemical Energy* (Eds. K. Swider-Lyons and C. Breitung, Springer) Chapter 27, 897 (2017).
- “Perovskite Proton Conductors for Energy Conversion and Storage at Intermediate Temperatures,” T. He and D. Ding, *20th Topical Meeting of the International Society of Electrochemistry*, Buenos Aires (March 2017), Oral.
- [“Hydrogen production via water electrolysis at intermediate temperatures,”](#) T. He and D. Ding, IDR # 4276, Patent Application filed (2017).



# Publications and Presentations

- “Covalent Surface Modification of GaAs(100) Photocathodes for Water Splitting in Highly Acidic Electrolyte,” Garner, L. E., Steirer, K. X., Young, J. L., Anderson, N. C., Miller, E. M., Tinkham, J. S., Deutsch, T. G., Sellinger, A., Turner, J. A. and Neale, N. R., *ChemSusChem*. **10**, 767-773 (2017).
- “Influence of support electrolytic in the electrodeposition of Cu-Ga-Se thin films,” A.M. Fernandez, J.A. Turner, B. Lara-Lara, T.G. Deutsch, *Superlattices and Microstructures* **101**, 373-383 (2017).
- “Employing Overlayers to Improve the Performance of Cu<sub>2</sub>BaSnS<sub>4</sub> Thin Film based Photoelectrochemical Water Reduction Devices,” Jie Ge, Paul J. Roland, Prakash Koirala, Weiwei Meng, James L. Young, Reese Petersen, Todd G Deutsch, Glenn Teeter, Randy J. Ellingson, Robert W. Collins, and Yanfa Yan, *Chem. Mater.* **29**(3), 916-920 (2017).
- “Direct solar-to-hydrogen conversion via inverted metamorphic multi-junction semiconductor architectures,” James L. Young, Myles A. Steiner, Henning Döscher, Ryan M. France, John A. Turner, and Todd G. Deutsch, *Nature Energy* **2**, 17028 (2017).
- “Printed assemblies of GaAs photoelectrodes with decoupled optical and reactive interfaces for unassisted solar water splitting,” Dongseok Kang, James L. Young, Haneol Lim, Walter E. Klein, Huandong Chen, Yuzhou Xi, Boju Gai, Todd G. Deutsch, and Jongseung Yoon, *Nature Energy* **2**, 17043 (2017).



# Technical Backup Slides

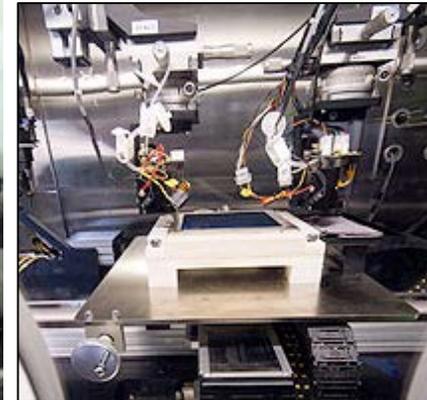
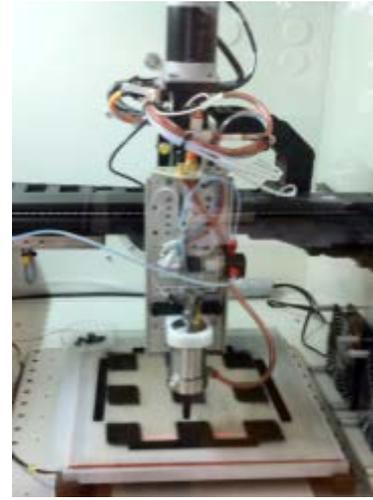


# Example Node: NREL High-Throughput Approaches to Scaling PEM Electrolysis Electrodes Using Relevant Production Technologies

LTE : CAT 1

## High-Throughput Scaling Concepts

- Important to understand scalability of new catalyst inks and electrode structures
  - Explore process-performance relationships
  - Explore pathways to low cost at high volume production
- Extend combinatorial aspect of EMNs by enabling gradient/matrixed electrode structures via scalable processes
  - Gradients can be in composition or structure
  - Gradients can be fabricated in X-Y or Z (thickness)



## Processing Capabilities

- Small-scale ink processing
  - Formulation, mixing, viscosity, rheometry
- Small-scale coating
  - Spin, knife, rod
- Spray coating
  - Ultrasonic, aerosol jet, ink jet, electro-spin/spray
- R2R coating
  - Slot die, micro-gravure



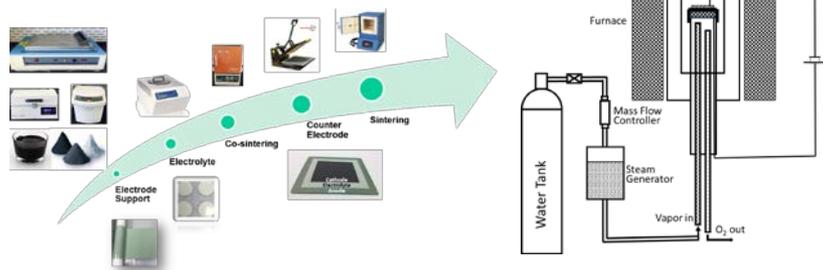
*Enable accelerated evaluation of electrode ink composition and properties as well as process parameters for optimal uniformity, performance, and durability*



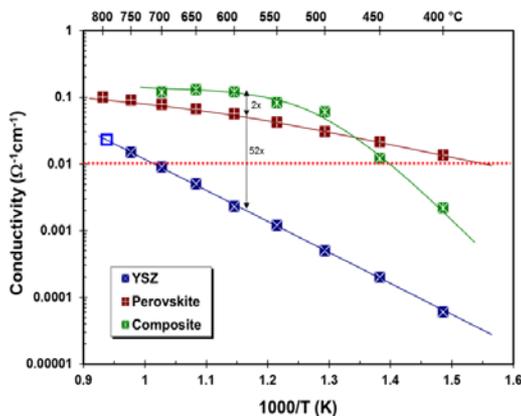
# Example Node: INL Advanced Materials for Water Electrolysis at Elevated Temperatures

HTE : CAT 2

## Cell Fabrication and Testing



## Advanced Electrolyte and Electrodes



**Purpose:** This node focuses on the development of advanced electrode and electrolyte materials for water electrolysis at intermediate temperatures (200°-600°C).

## INL's Key Features:

- Materials discovery, synthesis, characterization, and scale-up
- Cell fabrication and microstructure modification
- High-throughput performance testing and electrochemical characterization
- Advanced materials and structure characterization
  - Local Electrode Atom Probe
  - TEM/SEM/EDX
  - Chemical Analysis
  - Multidimensional and Multiphysics Modeling
  - Positron Annihilation Spectroscopy
- High temperature corrosion and materials stability analysis
  - Diffusion & Migration
  - Solid State Reaction

## Node Advantages

- Experts seek to improve ionic conductivity at intermediate temperatures by up to two orders of magnitude
- Lower operation temperature can reduce the chemical diffusion, migration, solid state reaction, corrosion, etc.
- Dry hydrogen, purification is not required
- Potential to eliminate Ni-catalysts oxidation by concentrated steam
- Avoid delamination due to high oxygen partial pressure at the interface operated at high current density



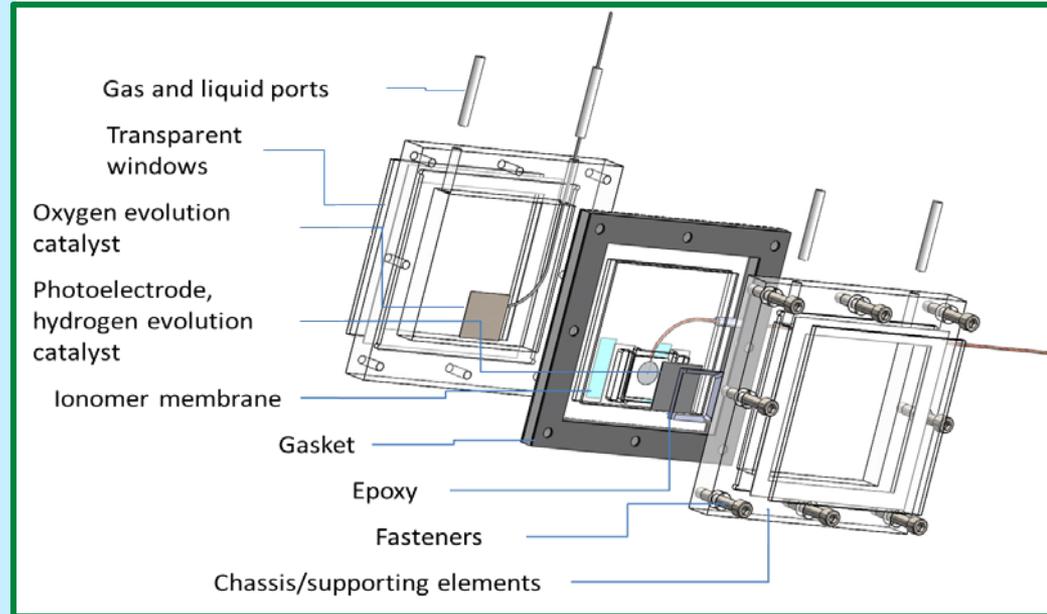


# Example Node: LBNL Photoelectrochemical Device Fabrication Facility

PEC : CAT 1

## Design and Fabrication

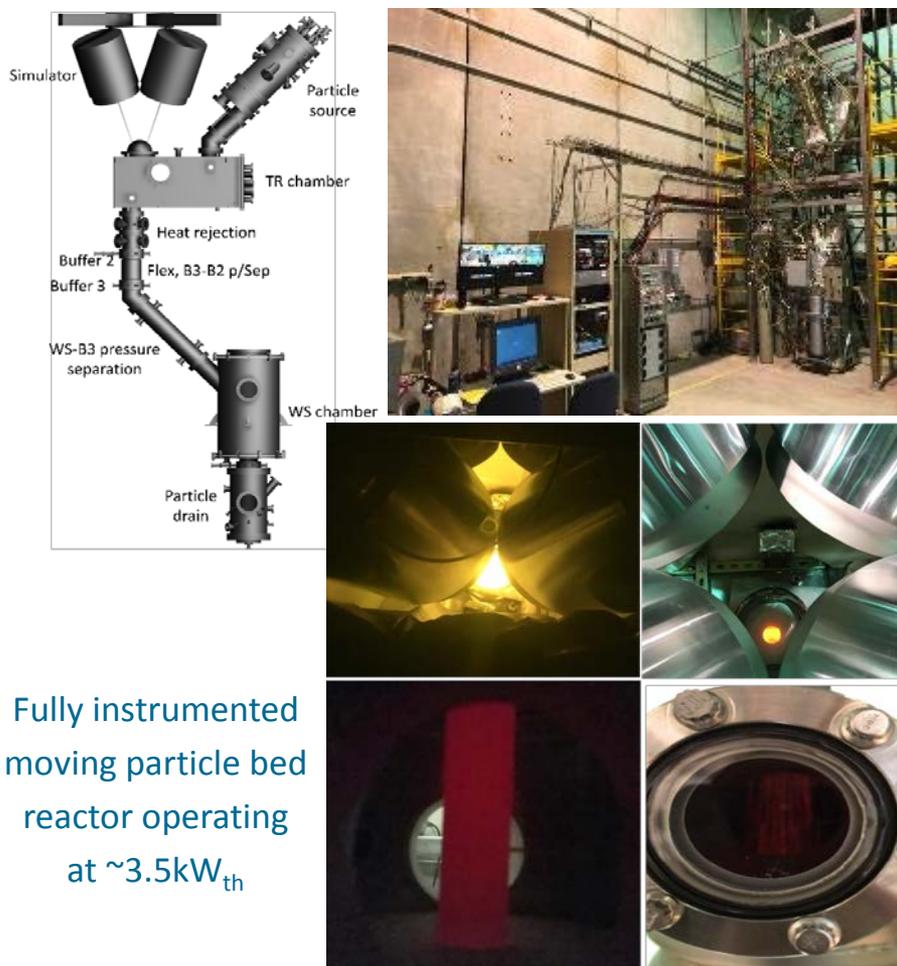
- Extensive expertise in designing and assembling cells
  - Guided by modeling
- Equipment
  - Connex 350 inkjet 3D-printer
    - Resolution 16 microns z-axis and 600 microns x-y axis
    - Working volume 30 x 30 x 30 cm
    - Printing materials: acrylic acrylates
  - Database for compatible materials plastics and epoxies
  - Custom tooling for mounting device components during assembly
  - Othermill milling machine
    - CAD to CAM software
    - Resolution 25 microns
    - Working volume 14x11.4x4.06 cm





# Example Node: SNL High Efficiency STCH Reactor

STCH : CAT 2



Fully instrumented  
moving particle bed  
reactor operating  
at  $\sim 3.5\text{kW}_{\text{th}}$

Purpose: The reactor is a kW-sized test device powered by simulated solar radiation designed to evaluate the performance of STCH materials under a wide range of relevant and realistic operating conditions.

## Key Features:

- $12\text{kW}_{\text{el}}$  ( $3.5\text{kW}_{\text{th}}$ ) solar simulator that can instantaneously generate peak solar concentrations greater than 1,000 suns over a  $30\text{ cm}^2$  aperture.
- Radiant cavity receiver operates at  $>1500^\circ\text{C}$ .
- Widely adjustable particle mass flow rate and receiver residence.
- Pressure and temperature separation in two-step cycle achieved by moving packed bed of particles.
  - $1700\times$  pressure separation
  - 100 kg redox-active material
  - $2.5\text{ g/s}$  particle flow rate
  - $0.3\text{ slpm H}_2$  continuous

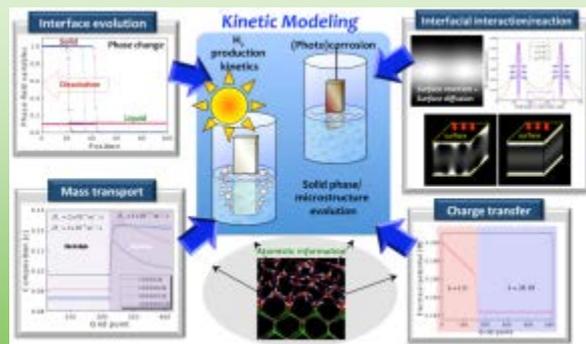
## References:

- I. Ermanoski, "Cascading Pressure Thermal Reduction for Efficient Solar Fuel Production", International Journal of Hydrogen Energy 39 (2014) 13114



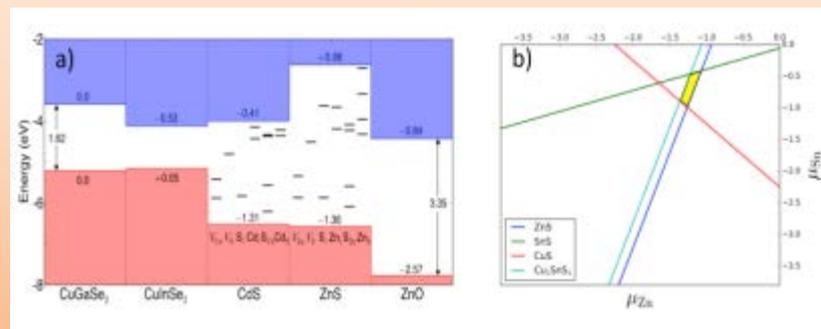
# Theory/Computational Capabilities (LLNL, LBNL, SNL, NREL)

## Simulating processes



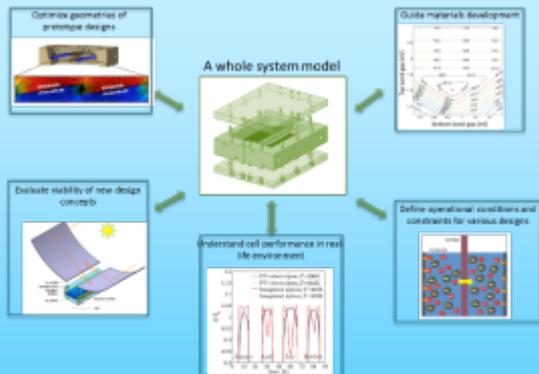
From atomistic to macroscopic

## Assisting material synthesis

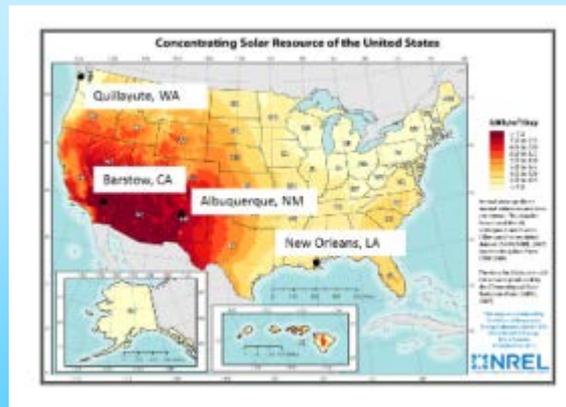


Materials design and diagnostics

## Predicting performance



Based on device design

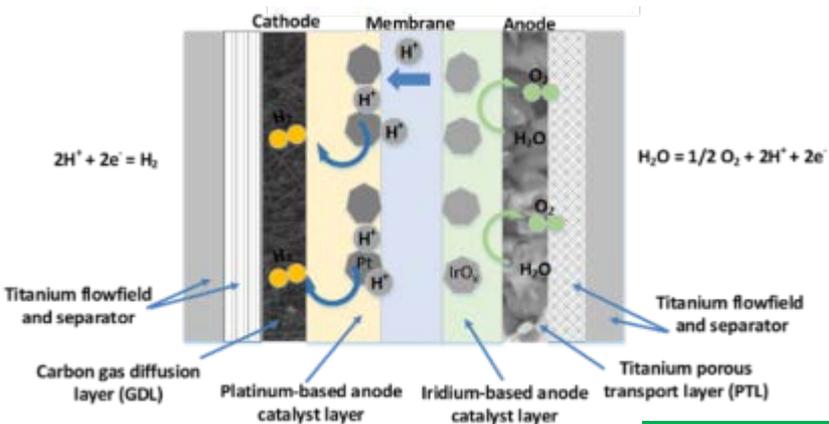


Based on geography/climate

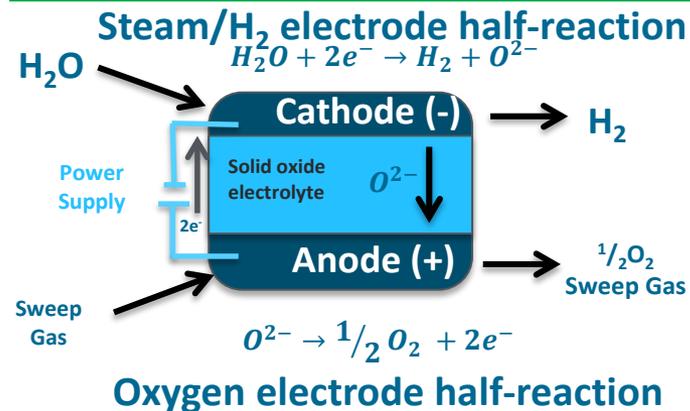


# Future Work – Explore Cross-Cutting Multiple Advanced Water Splitting Material (AWSM) Technologies

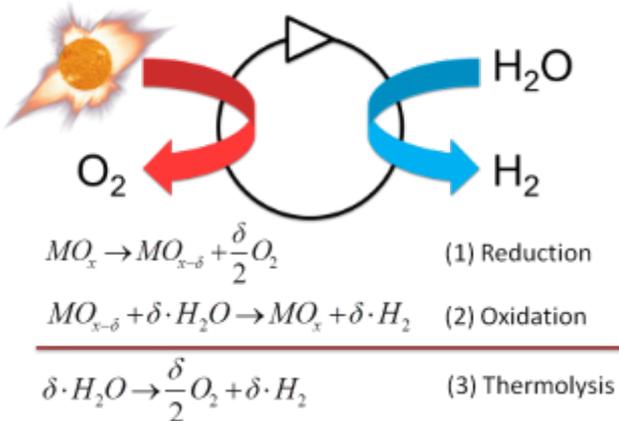
## PEM Electrolysis



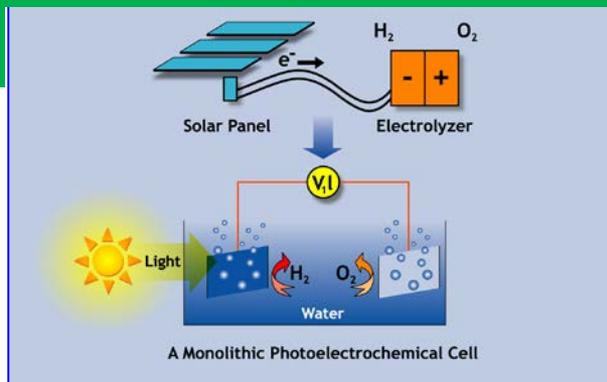
## Solid Oxide Electrolysis



## Solar Thermochemical



## Photoelectrochemical



## Hybrid Sulfur Cycle

