Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

# HydroGEN: A Consortium on Advanced Water Splitting Materials

H.N. Dinh, A. Weber, A. McDaniel, R. Boardman, T. Ogitsu, H. Colon-Mercado

Presenter: Huyen Dinh, NREL

Date: 6/8/2017

Venue: 2017 DOE Annual Merit Review

Project ID # PD148



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

# HydroGEN Overview

## Timeline and Budget

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

## Barriers

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

## Partners

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

BERKELEY LAB

Sandia National Laboratories

Lawrence Livermore National Laboratory

INL
Idaho National Laboratory

SRNL

# Advanced Water Splitting Materials Workshop April 2016 Stanford

**Assembled experts to identify cross-cutting research needs to accelerate materials discovery for sustainable $H_2$ production**

| Advanced Electrolysis | Photoelectrochemical | Solar Thermochemical |
|---|---|---|
| Low & High | | 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)

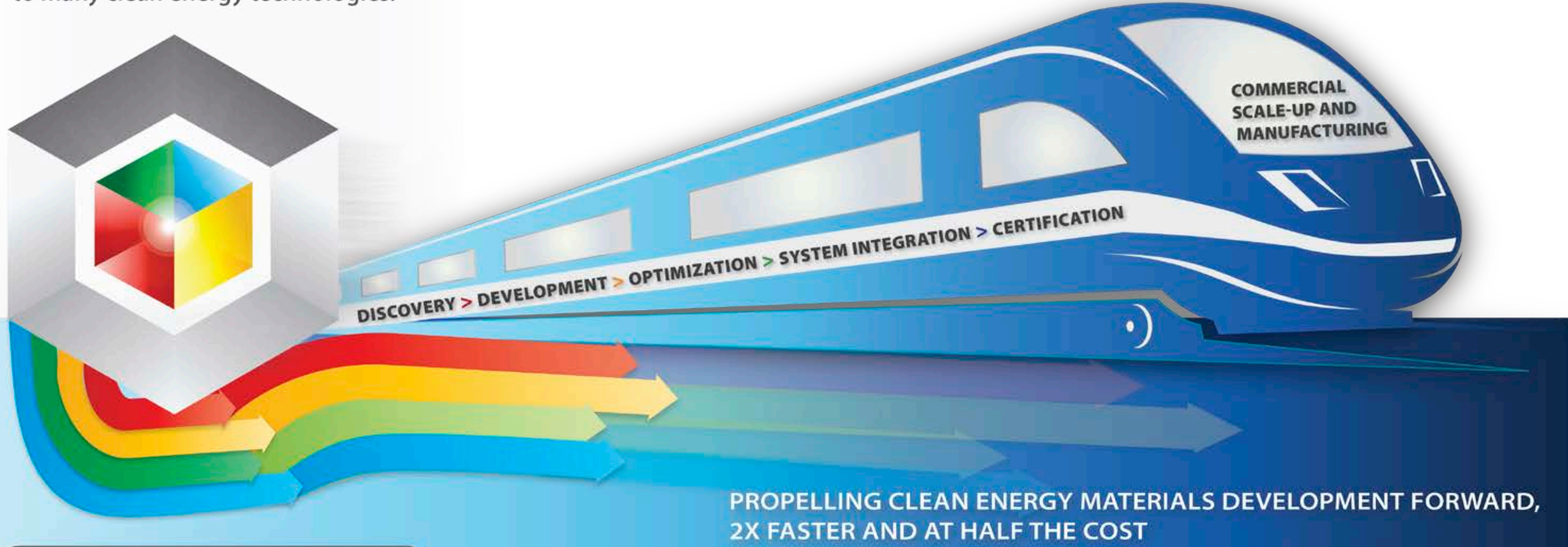
**Energy Materials Network**
U.S. Department of Energy

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

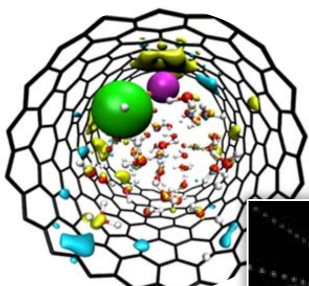
HydroGEN Advanced Water Splitting Materials

### Core Labs

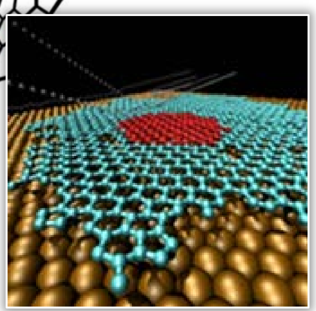
NREL National Renewable Energy Laboratory
Berkeley Lab
Sandia National Laboratories
INL Idaho National Laboratory
Lawrence Livermore National Laboratory
SRNL

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

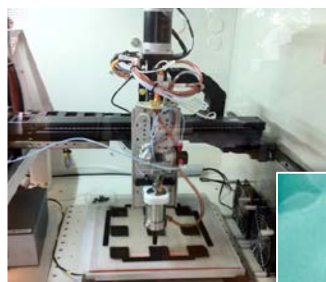
| ***Materials Theory/Computation*** | ***Advanced Materials Synthesis*** | ***Characterization & Analysis*** |
|---|---|---|



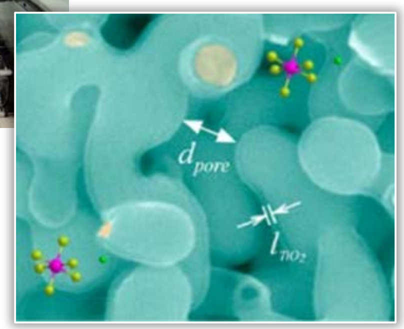
*Bulk and interfacial models of aqueous electrolytes*



*LAMMPS classic molecular dynamics modeling relevant to $H_2O$ splitting*

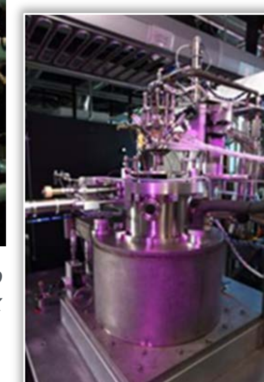


*High-throughput spray pyrolysis system for electrode fabrication*




*Conformal ultrathin $TiO_2$ ALD coating on bulk nanoporous gold*

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

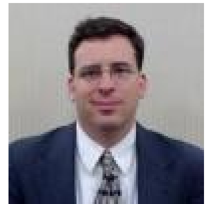


*TAP reactor for extracting quantitative kinetic data*

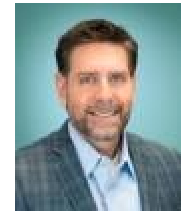
***HydroGEN fosters cross-cutting innovation using theory-guided applied materials R&D to advance all emerging water-splitting pathways for hydrogen production***

# 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**

**Meet biweekly via telecom/webcast**

# Collaborations: Established the HydroGEN Expert Teams

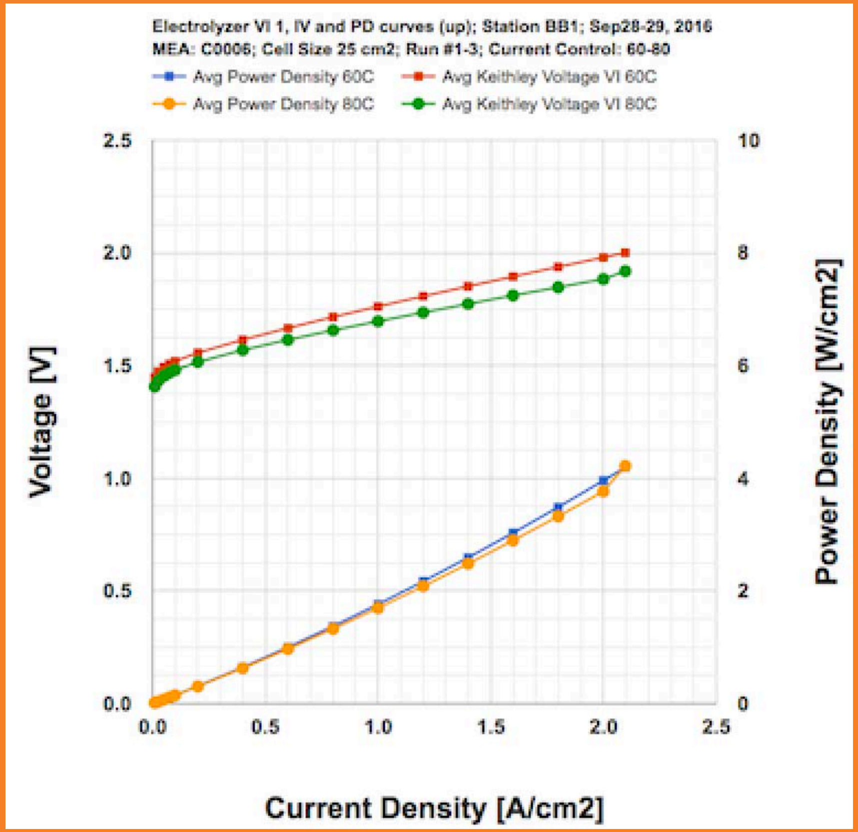
| Lab | Technical Experts | Data Experts | Technology Transfer Agreement (TT/A) Experts |
|---|---|---|---|
| NREL | Huyen Dinh | Kristin Munch, Robert White | Doreen Molk (IPMP, MTA), Eric Payne (IPMP), Megan Ballweber (NDA) Anne Miller (CRADA) |
| SNL | Anthony McDaniel | Richard Karnesky | Rachel 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) Benjaman 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

**Materials Transfer Agreement (MTA)**
- Freedom to Operate

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

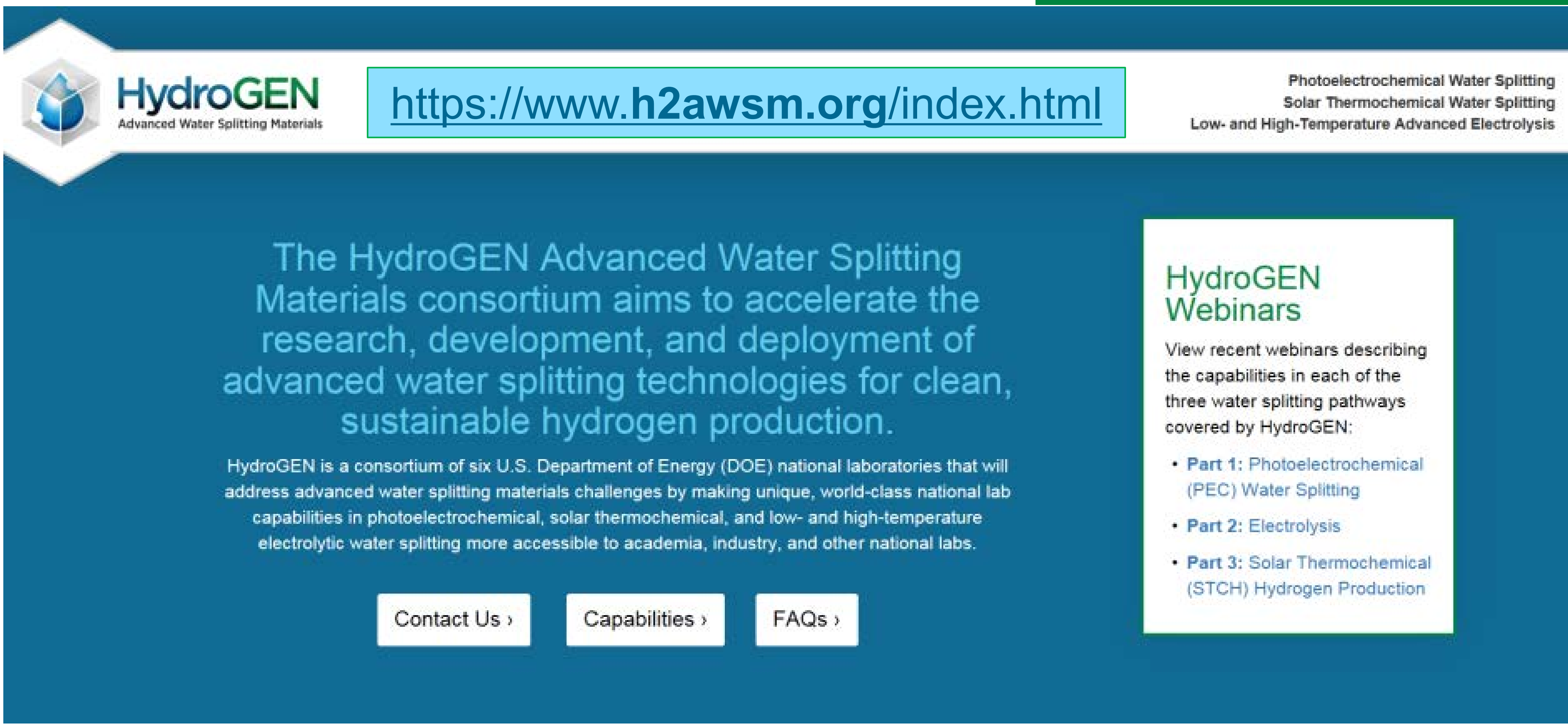
## ➢ Streamlined Access

- ➢ 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



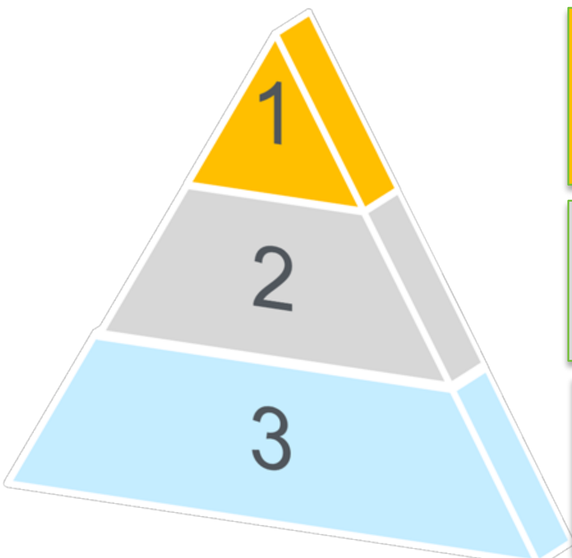

Users clicked on the HydroGEN contact email (mailto:h2awsm@nrel.gov) 285 times.

# 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



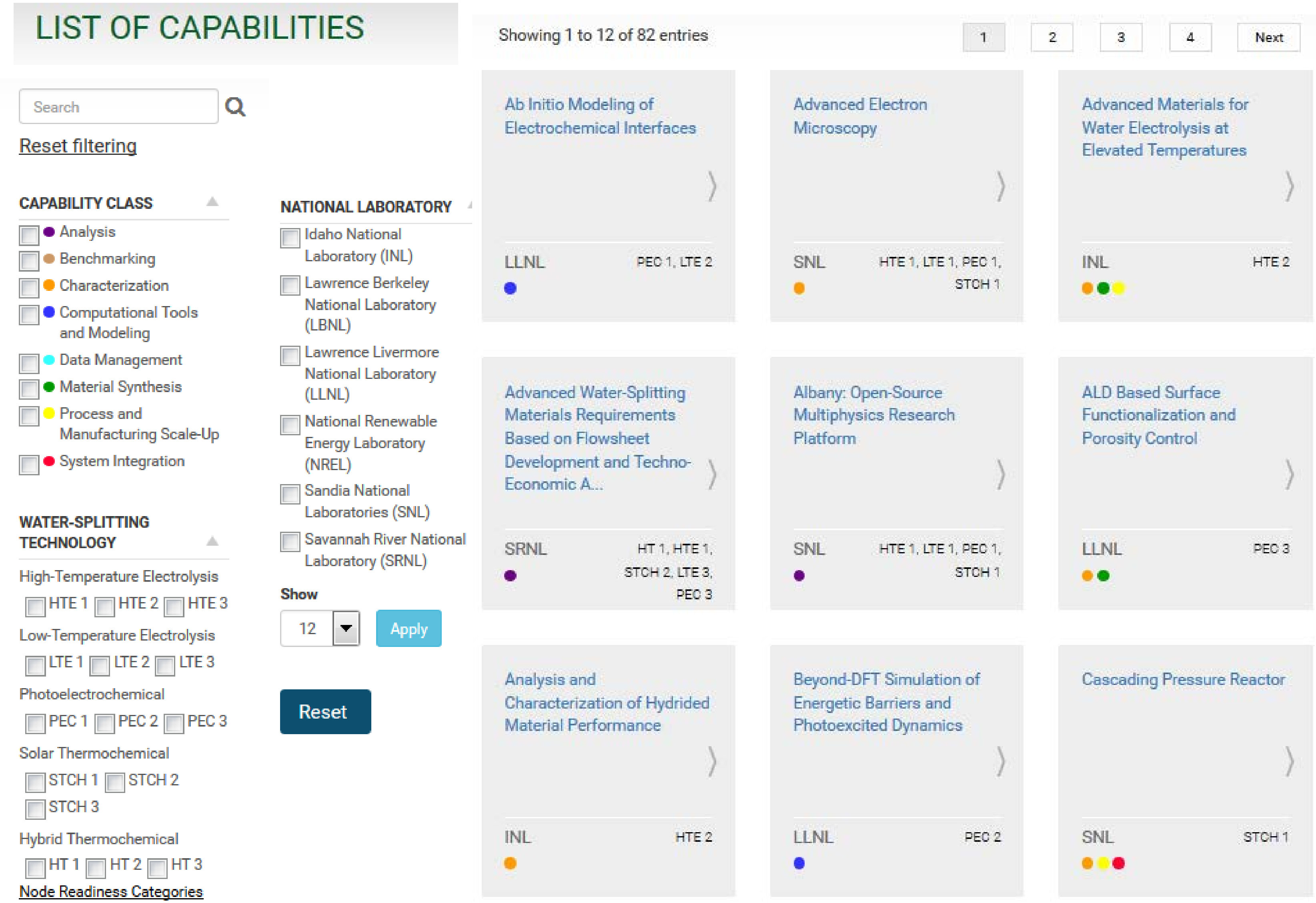

Category 1
Node is fully developed and has been used for AWSM research projects

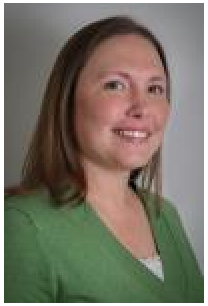
Category 2
Node requires some development for AWSM

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

# Accomplishments: New HydroGEN Website – Enhanced Capability Search



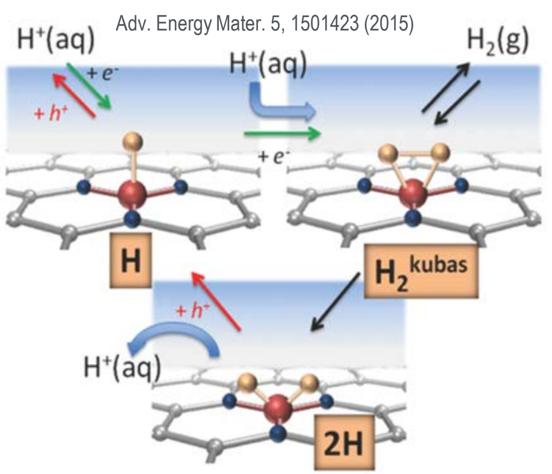



https://www.h2awsm.org/index.html

# 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***

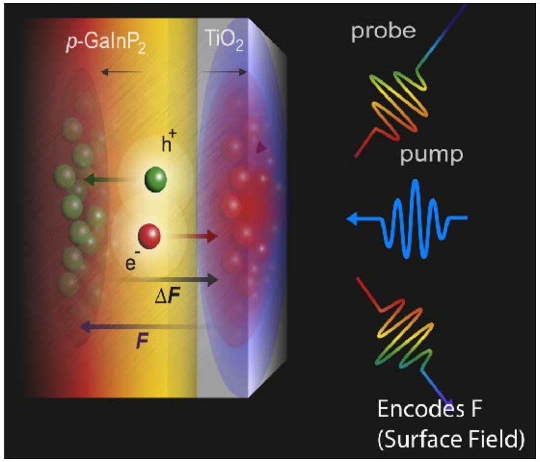



***Catalytic activity predictions using ab initio descriptors***

***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***

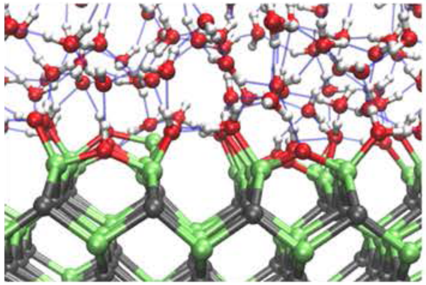
Several **nodes span multiple classification areas** (analysis, synthesis, characterization, etc.) **and different technologies** (AE, PEC, STCH)

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

**PEC : CAT 1**

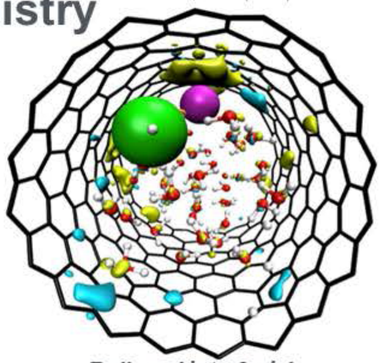
## Solid-liquid interfacial chemistry

JACS 135, 15774 (2013); Nat. Mater. (In press)



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

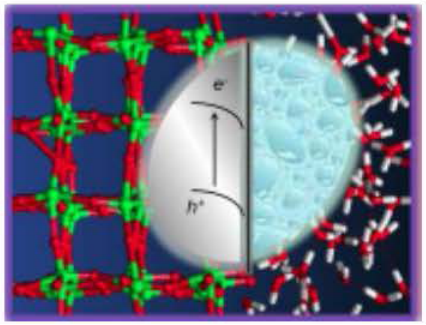
JPCC 120, 7332 (2016)



Bulk and interfacial properties of aqueous electrolytes

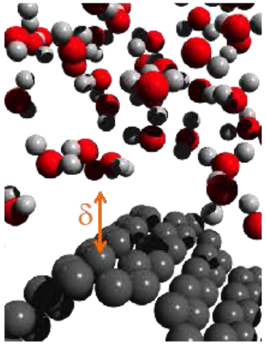
## Electronic properties of interfaces

JACS 136, 17071 (2014); PRB 89, 060202 (2014)




Electronic properties of electrode-electrolyte interfaces (from GW)

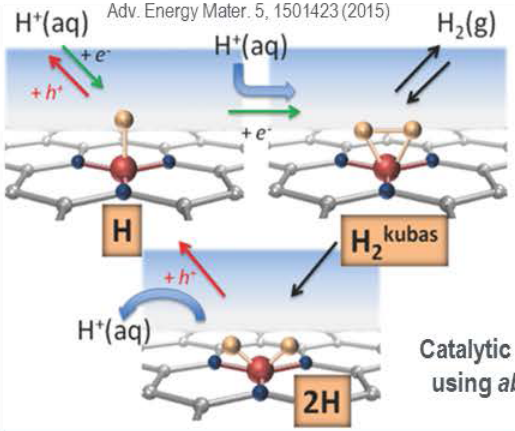
PRB 91, 125415 (2015); JPCC 118, 4 (2014)



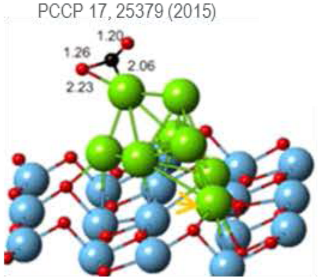

Simulations under applied bias or photobias

## Electrocatalysis and photocatalysis

Adv. Energy Mater. 5, 1501423 (2015)

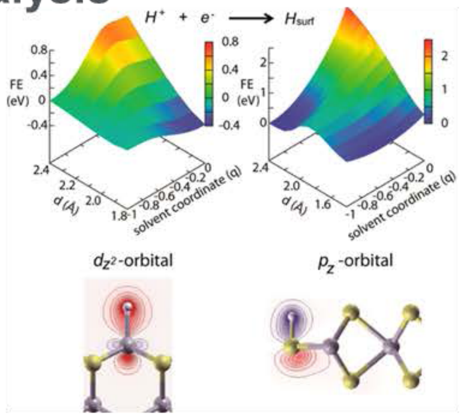



JPCC 118, 26236 (2014); PCCP 17, 25379 (2015)




Catalytic activity predictions using *ab initio* descriptors

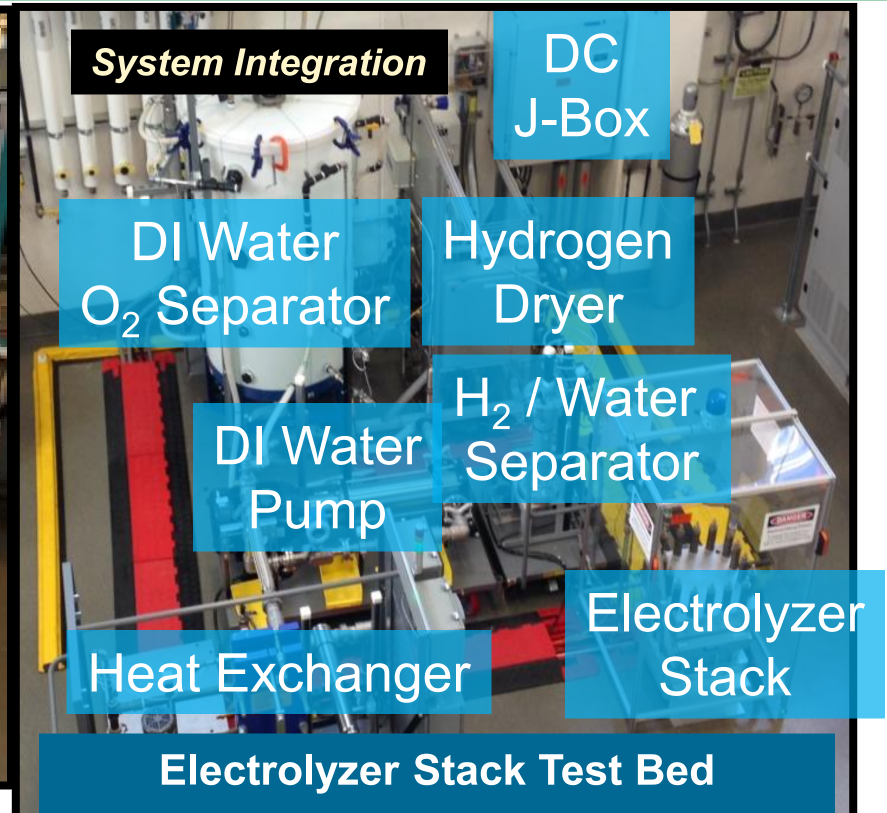
Charge-transfer barriers for $H_2$ evolution




JPCC 117, 21772 (2013)

# Example Node: NREL PEM Electrolyzer Testing Capabilities

**LTE : CAT 1**


## Greenlight Single Cell Test Systems

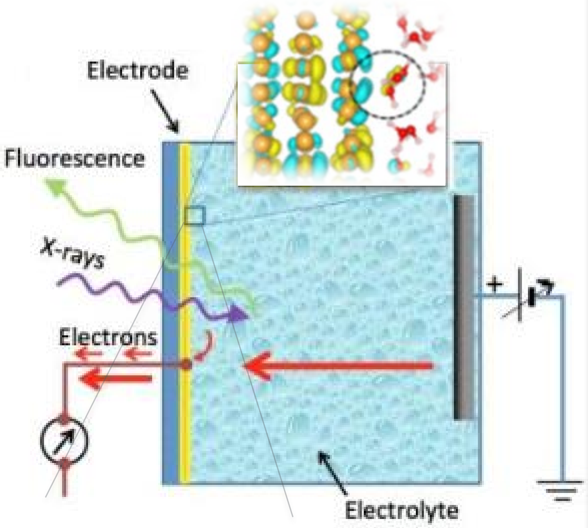
- 12V/250A power supply
- Up to 30 bar operation
- 5 cell voltage monitors
- AC impedance
- Anode and cathode product gas analyzer
- $H_2$ pump
- Up to 5 bar inlet pressure
- Up to 50 bar outlet pressure

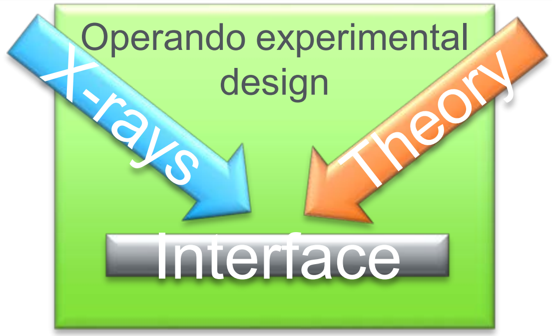
## Electrolyzer Stack Test Bed

- 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

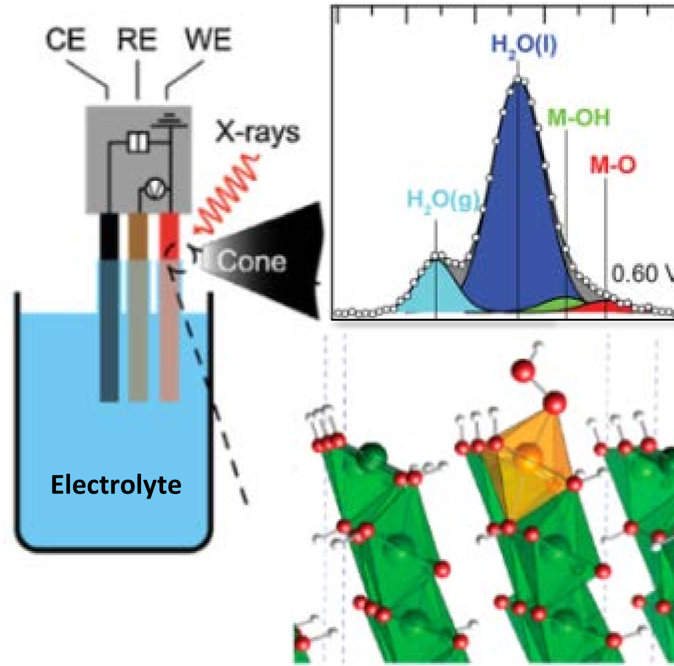
## Operando XAS

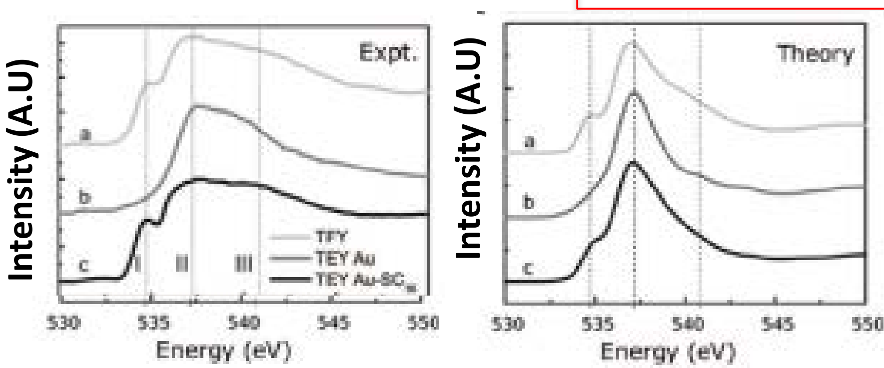



**Expertise combining operando instrumentation, X-ray spectroscopy, and theory to uncover molecular-scale chemical details at operating electrode interfaces**

## Operando ambient pressure XPS




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

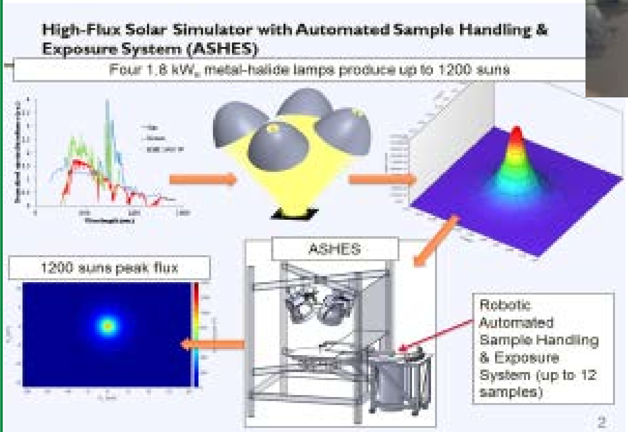
**X-ray absorption spectroscopy, coupled to theory, reveals electronic and atomic structure of chemical species at electrode interface**

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

**STCH, HT : CAT 1**

16 kW solar furnace

High-flux solar simulator

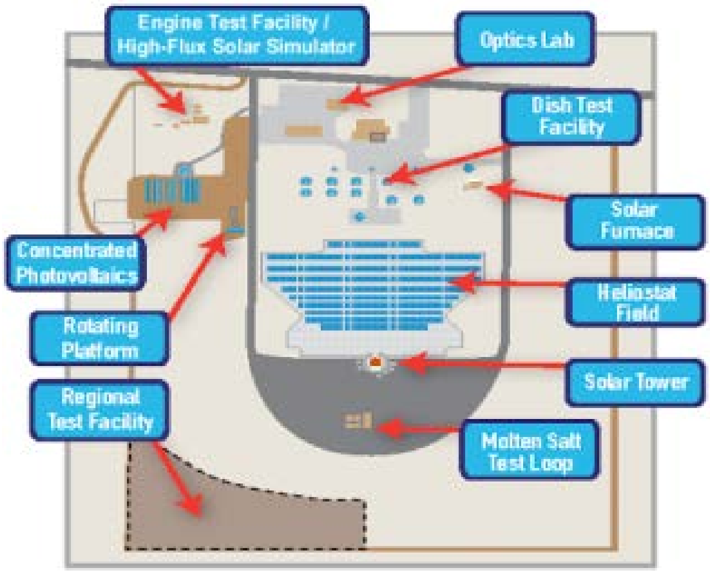



6 MW power tower

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.



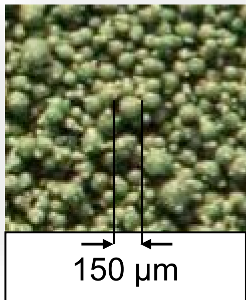

http://energy.sandia.gov/energy/renewable-energy/solar-energy/csp-2/nsttf/

# Example Node: INL Commissioned 2nd TAP Reactor for Quantification of Catalyst Kinetics

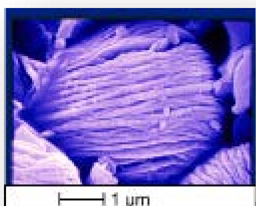
**HTE, STCH : CAT 2**

Industrial process

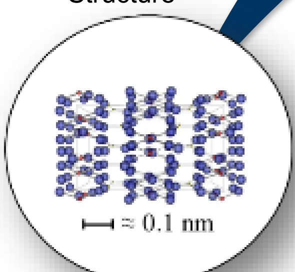

Spray dried catalyst form for attrition-resistant industrial use




SEM image of bulk catalyst particle with layered structure




$(VO)_2P_2O_7$ Crystal Structure




**Molecular scale chemistry**

**Catalyst scale-up and forming processes**

**Industrial scale manufacture**

***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**

Temporal Analysis of Products (pulse response technique)

Fundamental Kinetics of Industrial Catalysts Understood with TAP

Synthesis → Scale-up → Regeneration → Piloting

*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 $H_2$ 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

**Any proposed future work is subject to change based on funding levels**

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

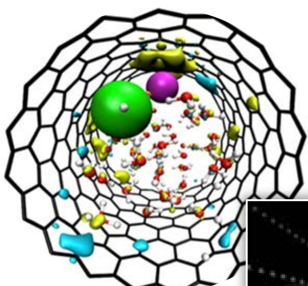
HydroGEN
Advanced Water Splitting Materials

## Core Labs

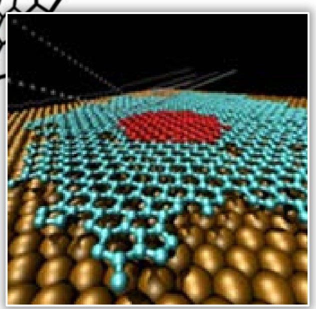
NREL – National Renewable Energy Laboratory
Berkeley Lab
Sandia National Laboratories
INL – Idaho National Laboratory
Lawrence Livermore National Laboratory
SRNL

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

### *Materials Theory/Computation*

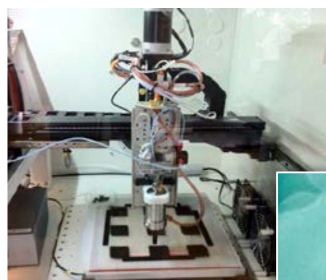


*Bulk and interfacial models of aqueous electrolytes*

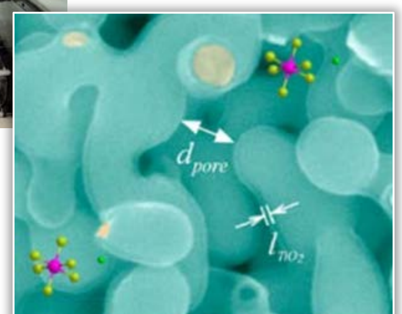


*LAMMPS classic molecular dynamics modeling relevant to $H_2O$ splitting*

### *Advanced Materials Synthesis*



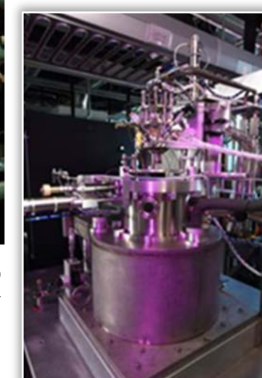
*High-throughput spray pyrolysis system for electrode fabrication*




*Conformal ultrathin $TiO_2$ ALD coating on bulk nanoporous gold*

### *Characterization & 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 |

## LBNL 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

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

# Acknowledgements

Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

## SNL Team

**Anthony McDaniel, Lead**
**Principal Investigators:**

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

## LLNL Team

**Tadashi Ogitsu, Lead**
**Principal Investigators:**

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

## INL Team

**Richard Boardman, Lead**
**Principal Investigators:**

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

NREL
BERKELEY LAB
Sandia National Laboratories
INL Idaho National Laboratory
Lawrence Livermore National Laboratory
SRNL

# 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) | **Complete Oct. 2016** |
| 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 **Modified to be due in April 2017 (Q3)** | QPM (Regular) | **Complete 4/20/2017** |
| Publish library of standardized HydroGEN NDA and CRADA forms. **(3 of 4 TT/A have been completed)** | 6/30/2017 | QPM (Regular) | **On Track** |
| 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) | **On Track** |

# 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 Photoelectrhemical 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. Breitkopf, 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 Cu2BaSnS4 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).

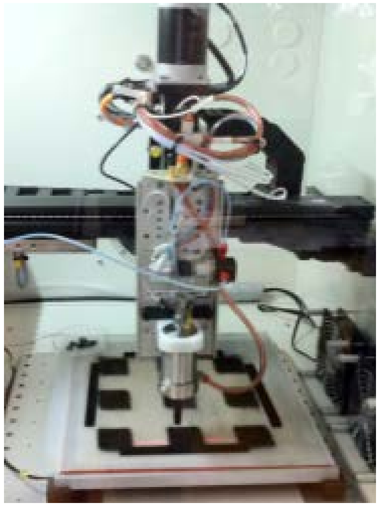
# Technical Backup Slides

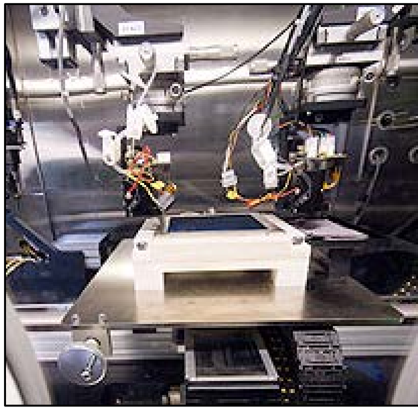
# Example Node: NREL High-Throughput Approaches to Scaling PEM Electrolysis Electrodes Using Relevant Production Technologies

**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

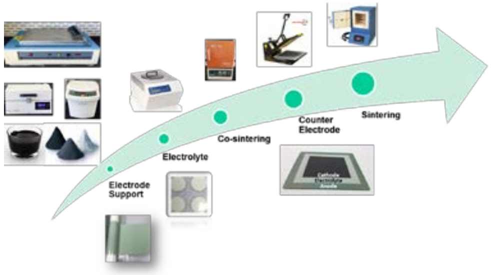
- Small-scale ink processing
  - Formulation, mixing, viscosity, rheometry
- Small-scale coating
  - Spin, knife, rod
- Spray coating
  - Ultrasonic, aerosol jet, ink jet, electro-spin/spray
- R2R coating
  - Slot die, micro-gravure

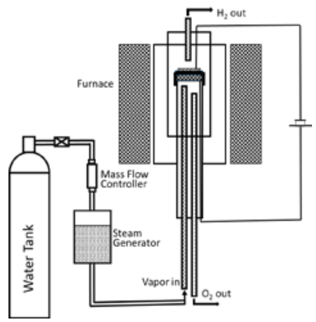
*Enable accelerated evaluation of electrode ink composition and properties as well as process parameters for optimal uniformity, performance, and durability*

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

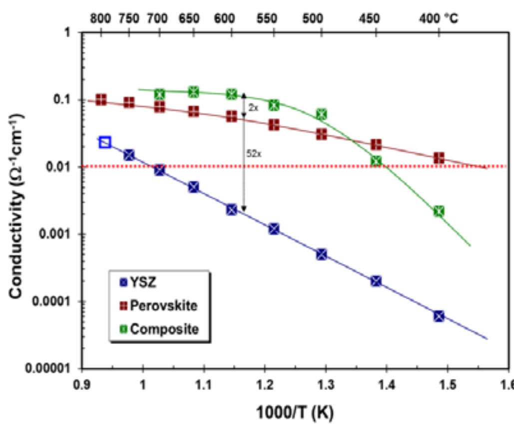
**HTE : CAT 2**

## Cell Fabrication and Testing




## Advanced Electrolyte and Electrodes




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

<u>INL's Key Features</u>:

- 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

<u>Node Advantages</u>

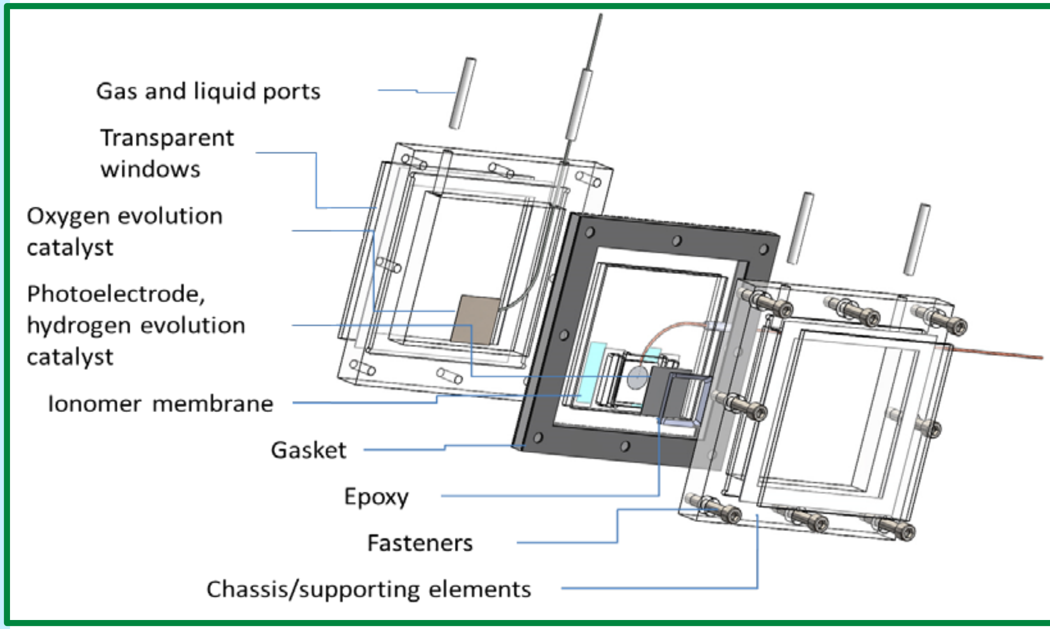
- Experts seek to improve ionic conductivity at intermediate temperatures by up to two orders of magnitude
- Lower operation temperature can reduce the chemical diffusion, migration, solid state reaction, corrosion, etc.
- Dry hydrogen, purification is not required
- Potential to eliminate Ni-catalysts 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**

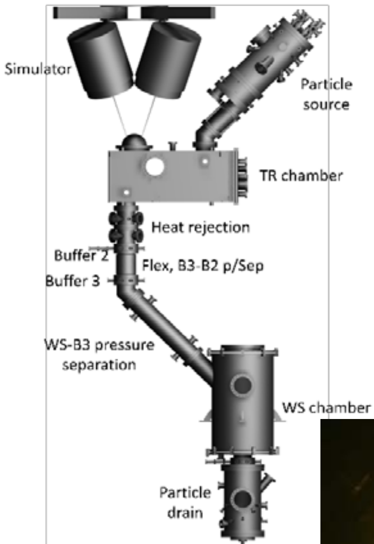
## Design and Fabrication

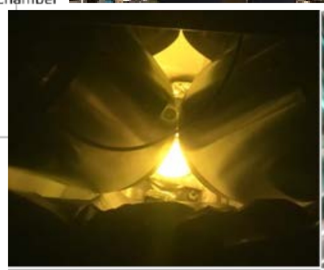
- Extensive expertise in designing and assembling cells
  - Guided by modeling
- Equipment
  - Connex 350 inkjet 3D-printer
    - Resolution 16 microns z-axis and 600 microns x-y axis
    - Working volume 30 x 30 x 30 cm
    - Printing materials: acrylic acrylates
  - Database for compatible materials 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

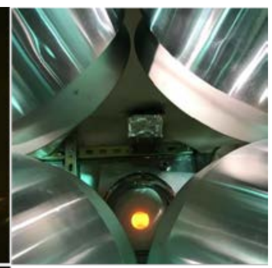


# Example Node: SNL High Efficiency STCH Reactor

**STCH : CAT 2**





Fully instrumented moving particle bed reactor operating at ~3.5kW$_{th}$

<u>Purpose</u>: 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.

<u>Key Features</u>:

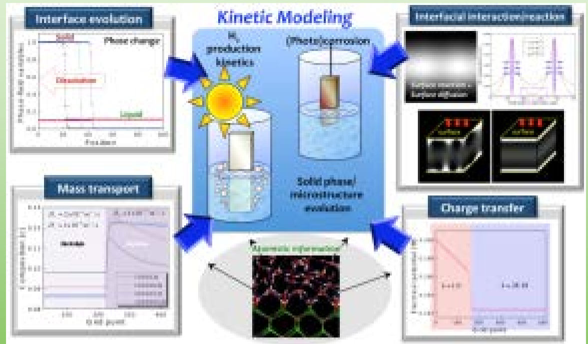
- 12kW$_{el}$ (3.5kW$_{th}$) solar simulator that can instantaneously generate peak solar concentrations greater than 1,000 suns over a 30 cm$^2$ aperture.
- Radiant cavity receiver operates at >1500°C.
- Widely adjustable particle mass flow rate and receiver residence.
- Pressure and temperature separation in two-step cycle achieved by moving packed bed of particles.
  - 1700× pressure separation
  - 100 kg redox-active material
  - 2.5 g/s particle flow rate
  - 0.3 slpm $H_2$ continuous

References:


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

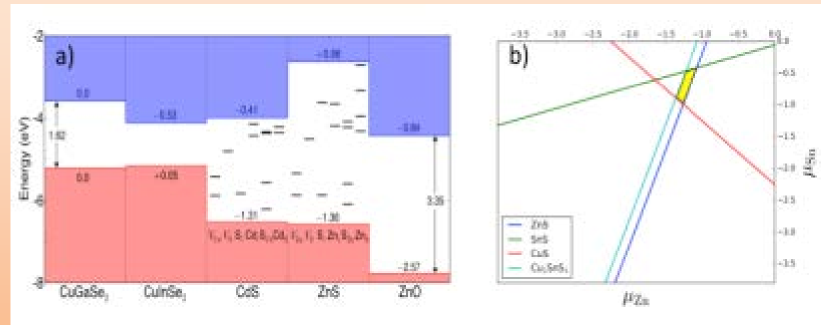
# Theory/Computational Capabilities (LLNL, LBNL, SNL, NREL)

## Simulating processes



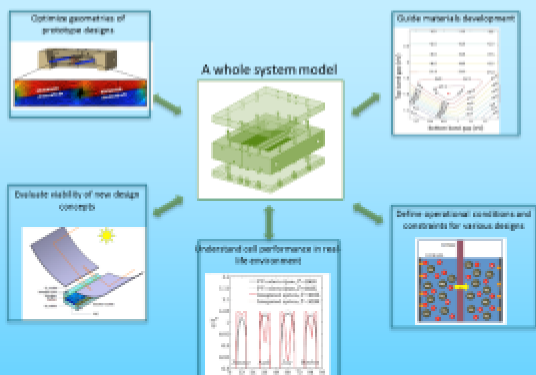

From atomistic to macroscopic

## Assisting material synthesis

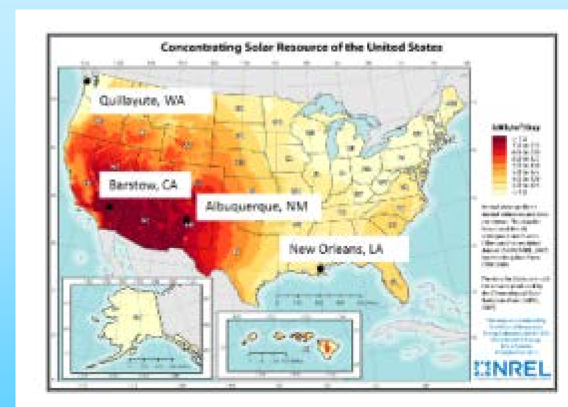



Materials design and diagnostics

## Predicting performance



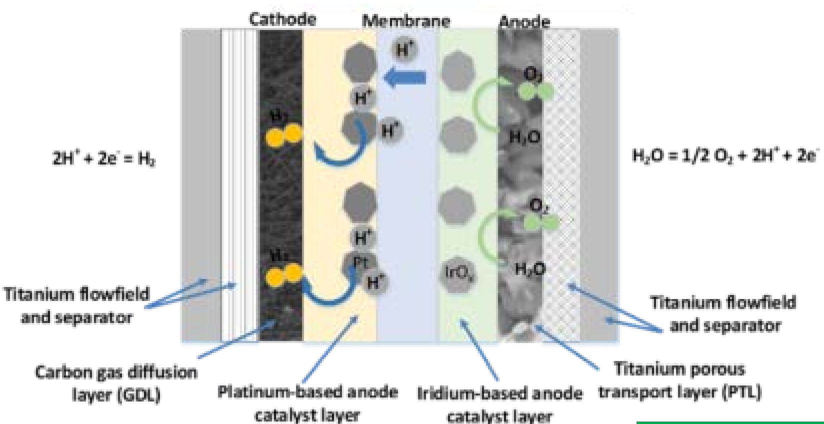

Based on device design




Based on geography/climate

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

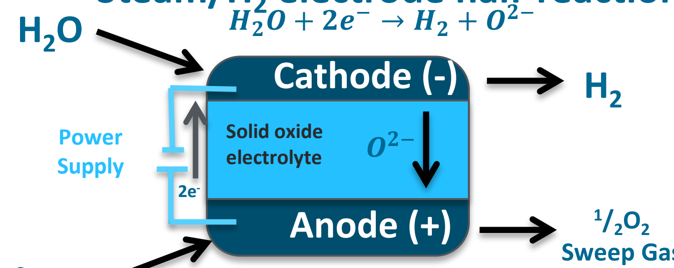
## PEM Electrolysis




## Solid Oxide Electrolysis

Steam/$H_2$ electrode half-reaction

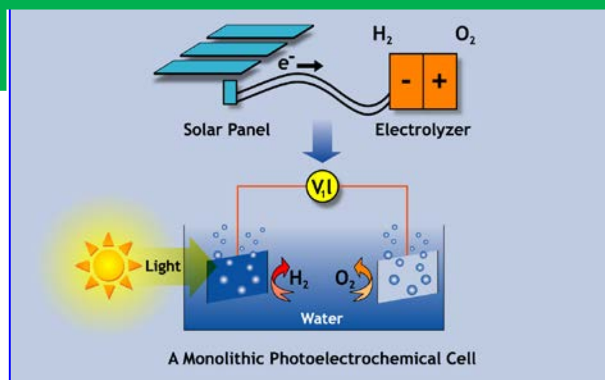
$$H_2O + 2e^- \rightarrow H_2 + O^{2-}$$



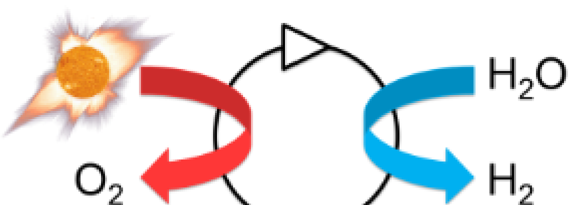

$$O^{2-} \rightarrow {}^{1}/_{2}\, O_2 + 2e^-$$

Oxygen electrode half-reaction

## Photoelectrochemical




## Solar Thermochemical




$$MO_x \rightarrow MO_{x-\delta} + \frac{\delta}{2} O_2 \quad \text{(1) Reduction}$$

$$MO_{x-\delta} + \delta \cdot H_2O \rightarrow MO_x + \delta \cdot H_2 \quad \text{(2) Oxidation}$$

$$\delta \cdot H_2O \rightarrow \frac{\delta}{2} O_2 + \delta \cdot H_2 \quad \text{(3) Thermolysis}$$

## Hybrid Sulfur Cycle