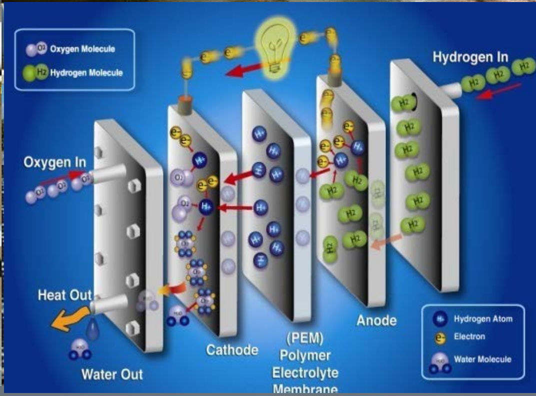
Fuel Cell Technologies Office Webinar

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy





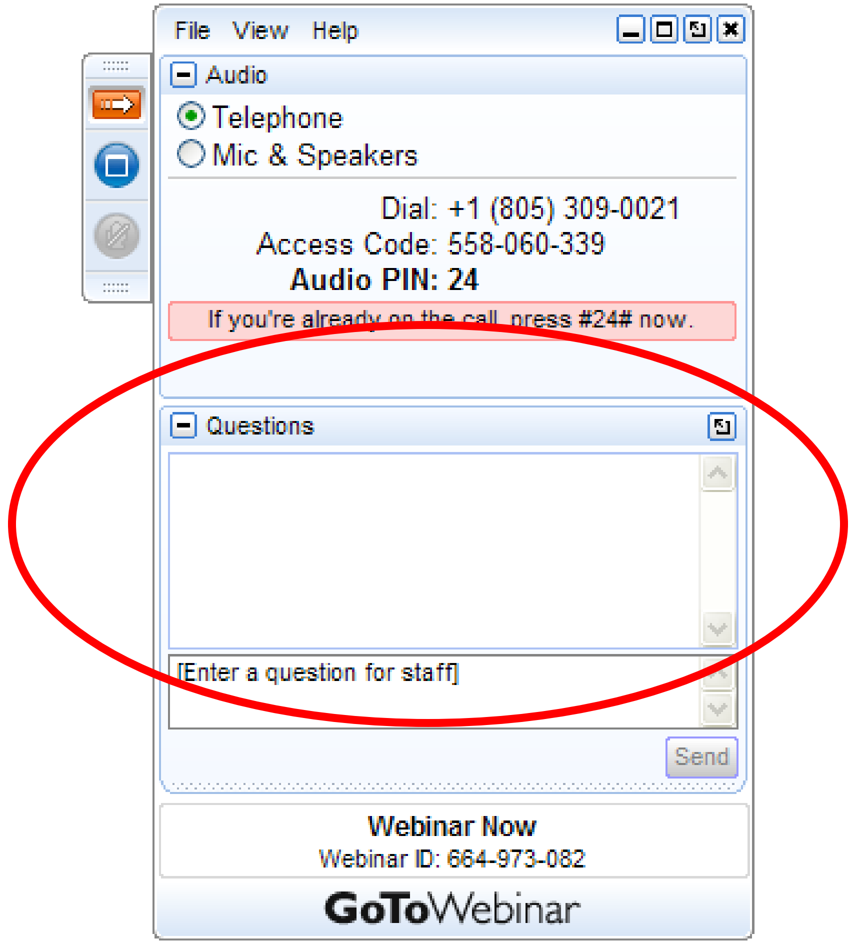
FCTO's HydroGEN Consortium Webinar Series, Part 2 of 3: Electrolysis

November 15, 2016

Huyen N. Dinh
Senior Scientist
HydroGEN Director

Question and Answer

- Please type your questions into the question box



Consortium Services

How do I find the right resource to accelerate a solution to my materials challenge?

How do I engage with the National Labs quickly and effectively?

The EMN offers a common yet flexible RD&D consortium model to address key materials challenges in specific high-impact clean energy technologies aimed at accelerating the tech-to-market process

HydroGEN Energy Materials Network (EMN)

Aims to accelerate the RD&D of advanced water splitting technologies for **clean, sustainable hydrogen production**, with a specific focus on **decreased materials cost**, **intermittent integration**, and **durability** *:*

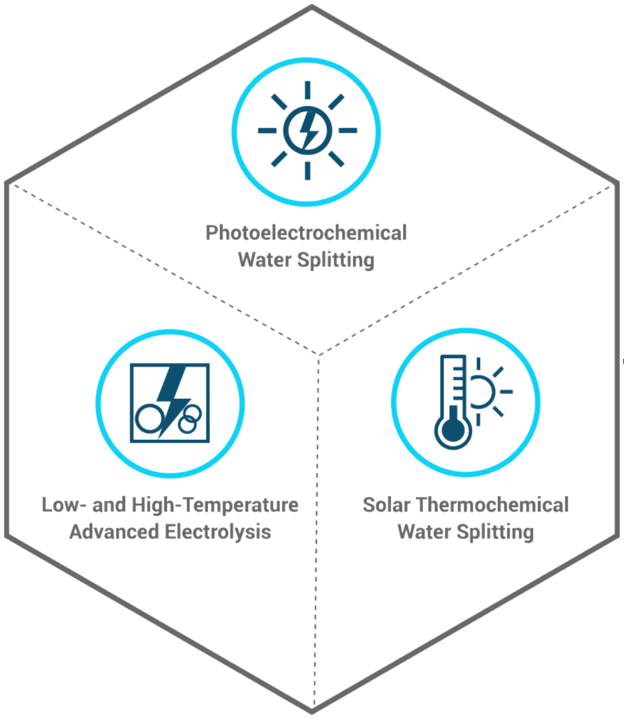
Advance Electrolysis	Photoelectrochemical	Solar Thermochemical
Low & High Temperature		Hybrid thermochemical

Major Outcomes from Stanford Workshop

- Detailed technoeconomic (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; and
  - **membranes/separations materials** research is needed for all technologies

Establish HydroGEN EMN consortium on Advanced Water Splitting Materials

RD&D from different water splitting pathways is critical to reducing renewable H_2 production cost



Production target <$2/gge

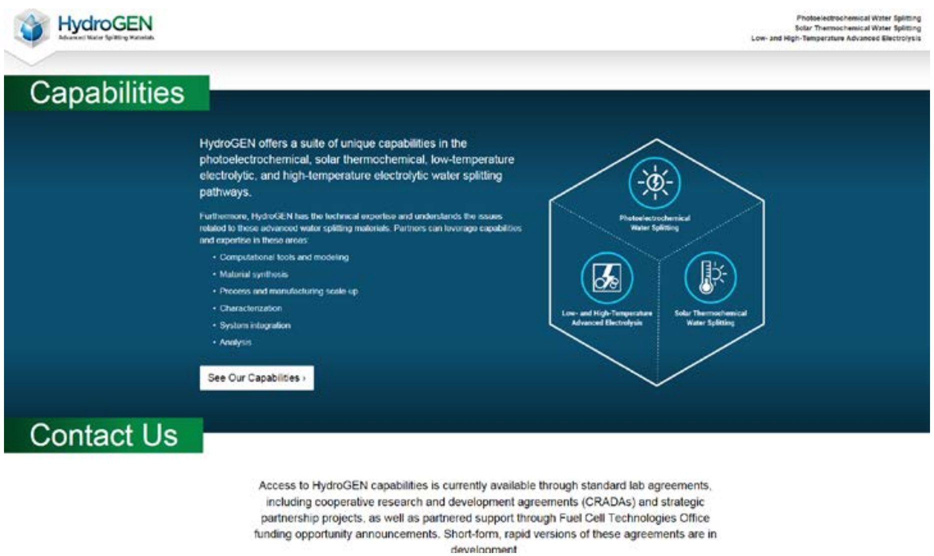
H_2 Cost at Pump

<$4/gge

<$7/gge (early market)

Technology Abbreviations:

- AE: Advanced Electrolysis
  - LTE: Low-Temperature Electrolysis
  - HTE: High-Temperature Electrolysis
  - HT: Hybrid Thermochemical
- PEC: Photoelectrochemical
- STCH: Solar Thermochemical

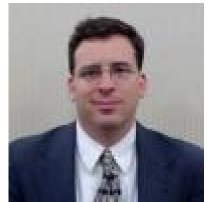


https://www.h2awsm.org/

HydroGEN Steering Committee

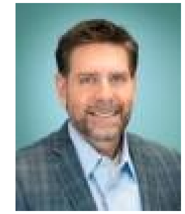
NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Huyen Dinh



BERKELEY LAB

Adam Weber



Sandia National Laboratories

Anthony McDaniel

INL
Idaho National Laboratory

Richard Boardman

Lawrence Livermore National Laboratory

Tadashi Ogitsu

SRNL
SAVANNAH RIVER NATIONAL LABORATORY

Héctor Colón-Mercado

Eric Miller, DOE-EERE-FCTO

Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

Part 2 of 3: Advanced Electrolysis

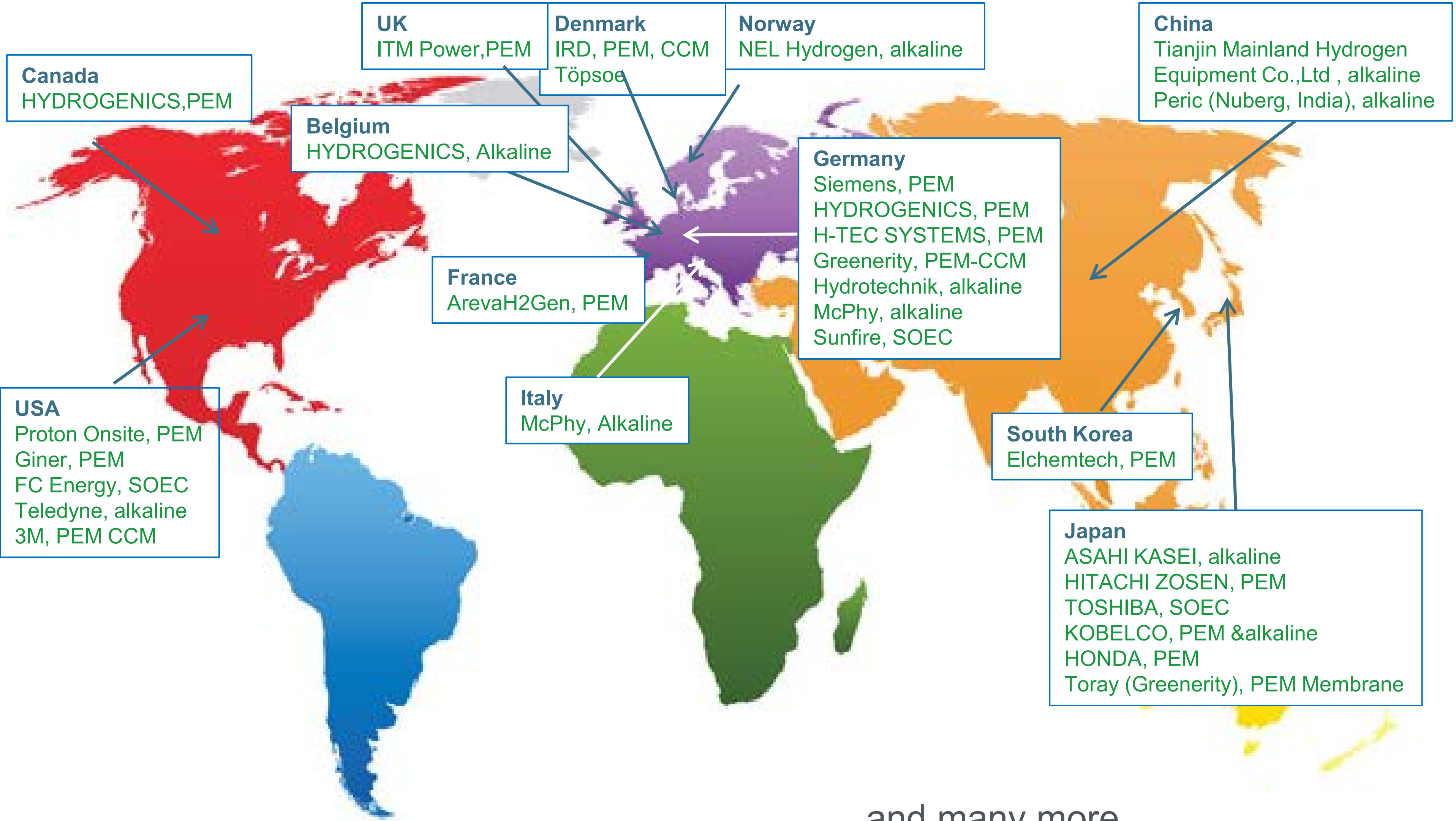
Huyen N. Dinh, Adam Weber, Richard Boardman, Tadashi Ogitsu, Héctor Colón-Mercado, Anthony McDaniel

November 15, 2016

FCTO Webinar

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

Main players in water electrolysis - 2016

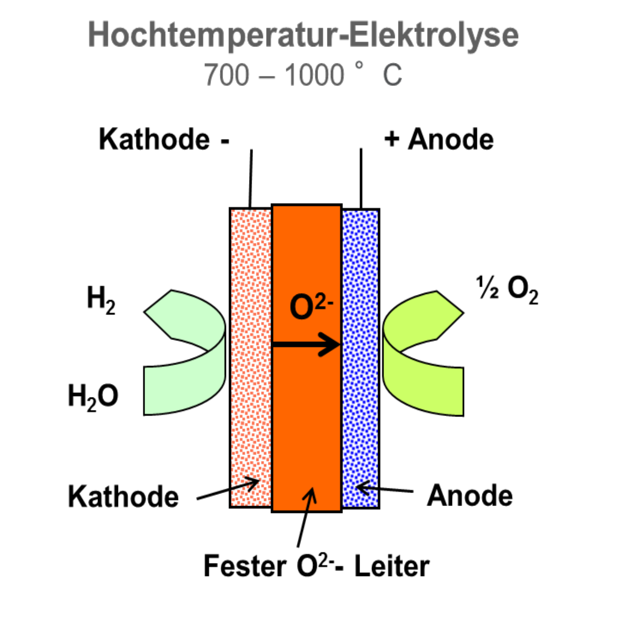


and many more….

Courtesy of M. Carmo, Julich, “Overview of latest developments in water electrolysis”, IEA Annex 30 Electrolysis, October 20-21 2016.

Water Electrolysis
- Solid Oxide Electrolysis (SOECs)

It has great potential for the future stationary hydrogen production (heat surplus), but still dependent on strong R&D activities (**durability (thermomechanical aspect)**)



$O^{2-} \rightarrow \frac{1}{2} O_2 + 2e^-$		Anode
$H_2O + 2e^- \rightarrow H_2 + O^{2-}$		Kathode
$H_2O \rightarrow H_2 + \frac{1}{2} O_2$		Gesamtreaktion

sunfire

SUNFIRE delivers the world largest commercially available reversible SOFC/SOFC system to Boeing

Electrolyse-Mode: 160 kW_{el}
Hydrogen: 42 Nm^3/h
Fuel Cell-Mode: 50 kW_{el}

Source: Press Release Sunfire GmbH, 23.02.2016

TOSHIBA
Leading Innovation

SOEC at hydrogen research and development center at Toshiba's Fuchu plant in Tokyo

Source: TOSHIBA

Courtesy of M. Carmo, Julich, "Overview of latest developments in water electrolysis", IEA Annex 30 Electrolysis, October 20-21 2016.

Scale-up towards MW systems
- PEM Electrolysis

HYDROGENICS, Canada & Deutschland
- E 1.500 Series Stacks: 1,5 MW
  30 bar, 150 % Peak

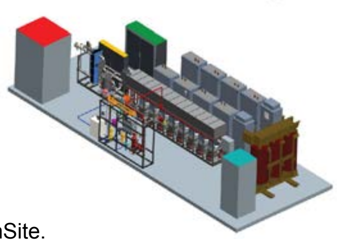
Source: HYDROGENICS

SIEMENS, Deutschland
- SILYZER 200, 1,25 MW
  35 bar, (2 MW Peak)

Source: Siemens

Proton OnSite, USA
- M Series PEM System
  M200 (200 Nm^3/hr) 4 Stacks, 1 MW
  M400 (400 Nm^3/hr) 8 Stacks, 2 MW

M Series M400 – 2 MW General Arrangement



Source: ProtonOnSite.

ITM Power, GB
- HGas1000, 16 Stacks, 1 MW
- 1 MW Stack Platform introduced at the Hannover Fair 2015

Source: ITM POWER.

Courtesy of M. Carmo, Julich, “Overview of latest developments in water electrolysis”, IEA Annex 30 Electrolysis, October 20-21 2016.

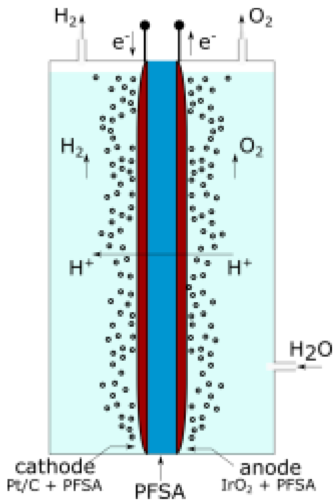
Main technical challenges for PEM water electrolyzers

- **Improve stack performance (efficiency) mainly related to:**
  - reduction of Ti dependence (bipolar plates and porous transport layers),
  - Membrane/Diaphragm (thin, reduced crossover, mechanical stability)
  - Catalysts
    - PEM: Oxygen Evolution reaction (IrO_x loading)

- **Dynamics, Flexibility, Start-up**

- **Pressure operation**

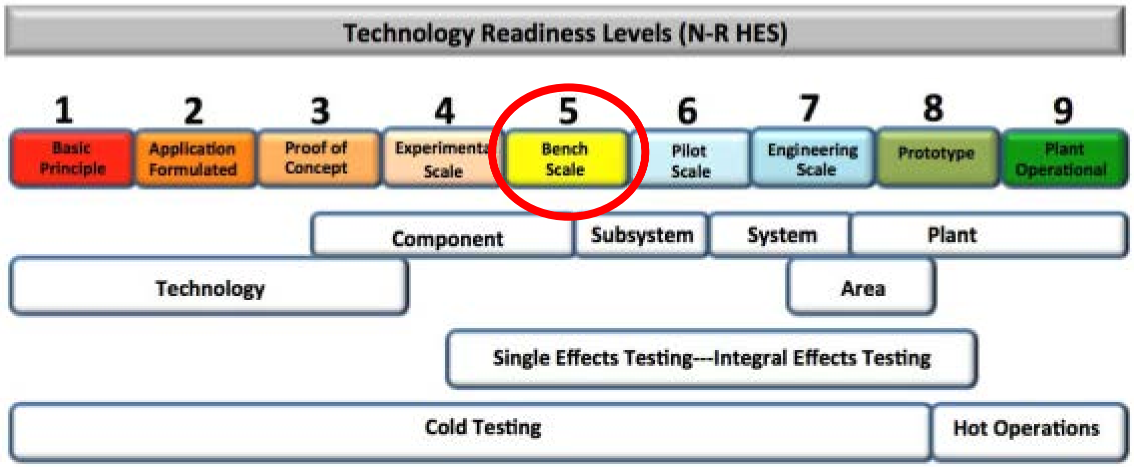
RELIABLE AND ROBUST !
> 50,000 hours



Courtesy of M. Carmo, Julich, "Overview of latest developments in water electrolysis", IEA Annex 30 Electrolysis, October 20-21 2016.

Current Status of High Temperature Electrolysis Technology

- International interest (US, Germany, Denmark, Canada, UK, China, …)
- State-of-the-art stacks demonstrate degradation rates < 3%/1000 hours
- State-of-the-art stacks claim survival of multiple thermal cycles
- Technology Readiness Level 5 (transition from experiment-scale to pilot-scale)



- Largest conducted demonstrations are beyond bench scale (10 kW) and approaching pilot scale (~100 kW or larger)
- 5 kW has evolved into one "standard" for module size
- Some performance testing on HTE in load following (electrical coupling)
- No demonstration on load following with electrical and thermal coupling
- Underdeveloped SOEC manufacturing processes / performance testing

High Temperature Steam Electrolysis R&D Needs

- Technoeconomic analysis of needs
  - Better (more defensible) estimates for nth of a kind electrolyzer cost
  - Defensible targets for HTE operational lifespan
  - Larger scale data for HTE operation in load following mode
    - Reversibility
    - Thermal management
    - Ramp rate
- Imbedded controls for dynamic operation and health monitoring
- Refine / standardize testing protocols for single-cells, single stacks, and multi-stack systems
- Understand water feedstock purity requirements
- Define and promote codes and standards relevant to High Temperature Electrolysis:
  - High temperature / high pressure H_2 and O_2 handling, storage
  - Quality control and performance metrics for cell manufacturing
  - Safety during normal and abnormal operations
- Resolution of technology scale-up issues
  - Parametric analysis to understand impacts of
    - cell size
    - number of repeat units
    - electrical and gas interconnect complexity
    - number of pressure vessels
  - Maintainability

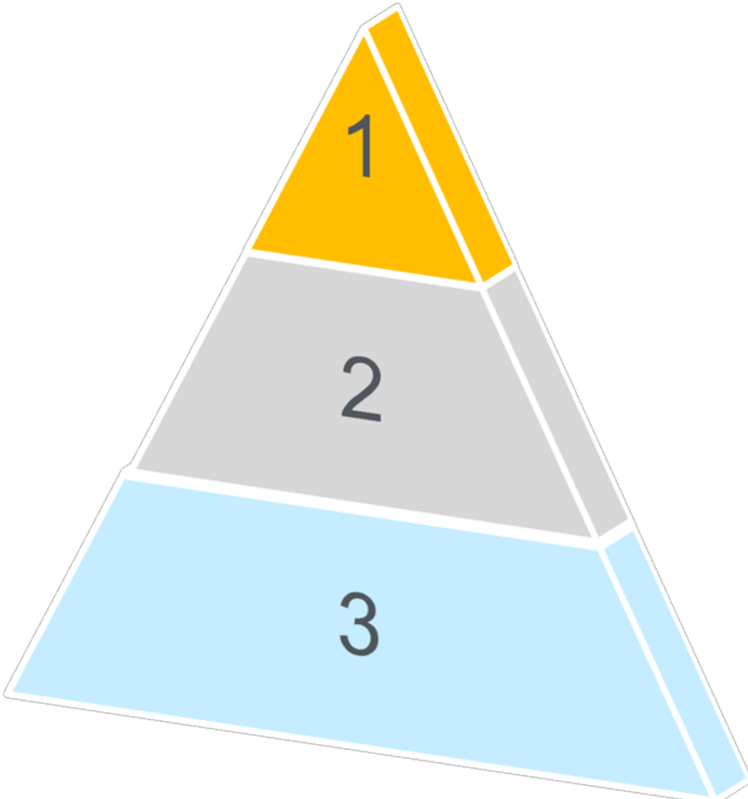
HydroGEN Capabilities Overview

Overall, there are about 80 capability nodes from 6 different labs:

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

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

Capability Node Readiness Category Chart



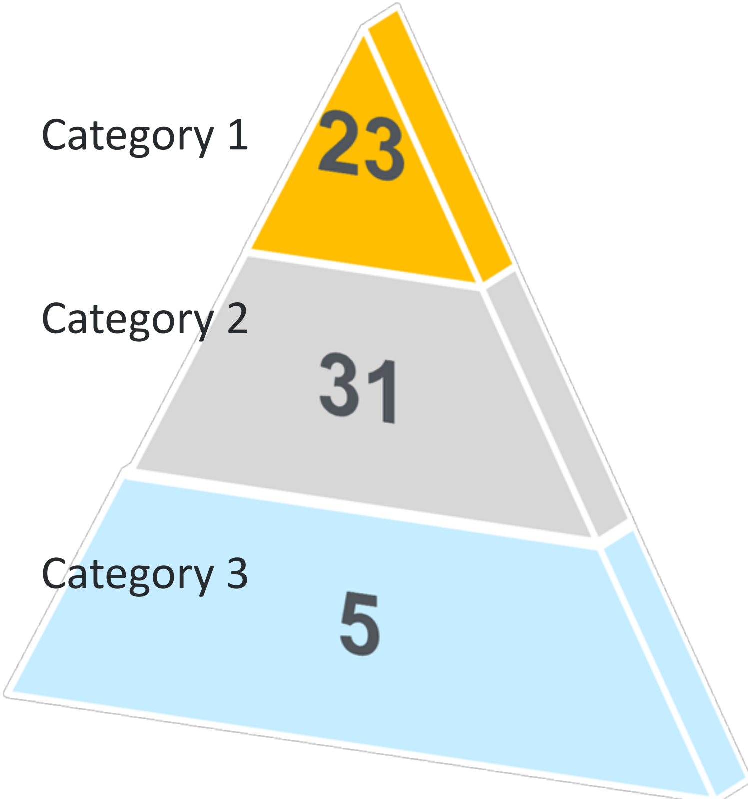
Category 1
Node is fully developed and has been used for AE research projects

Category 2
Node requires some development for AE

Category 3
Node requires significant development for AE

- **Nodes** comprise **tool, technique, and expertise** including **uniqueness**
- **Category** refers to **availability, readiness and relevance** to AE and not necessarily the expense and time commitment

59 Advanced Electrolysis (AE) Capability Nodes



Classification:

Category 1

Analysis: 2	**Characterization: 9**
Computation: 7	**Synthesis: 3**
System Integration: 1	**Process/Scale up: 1**

Category 2

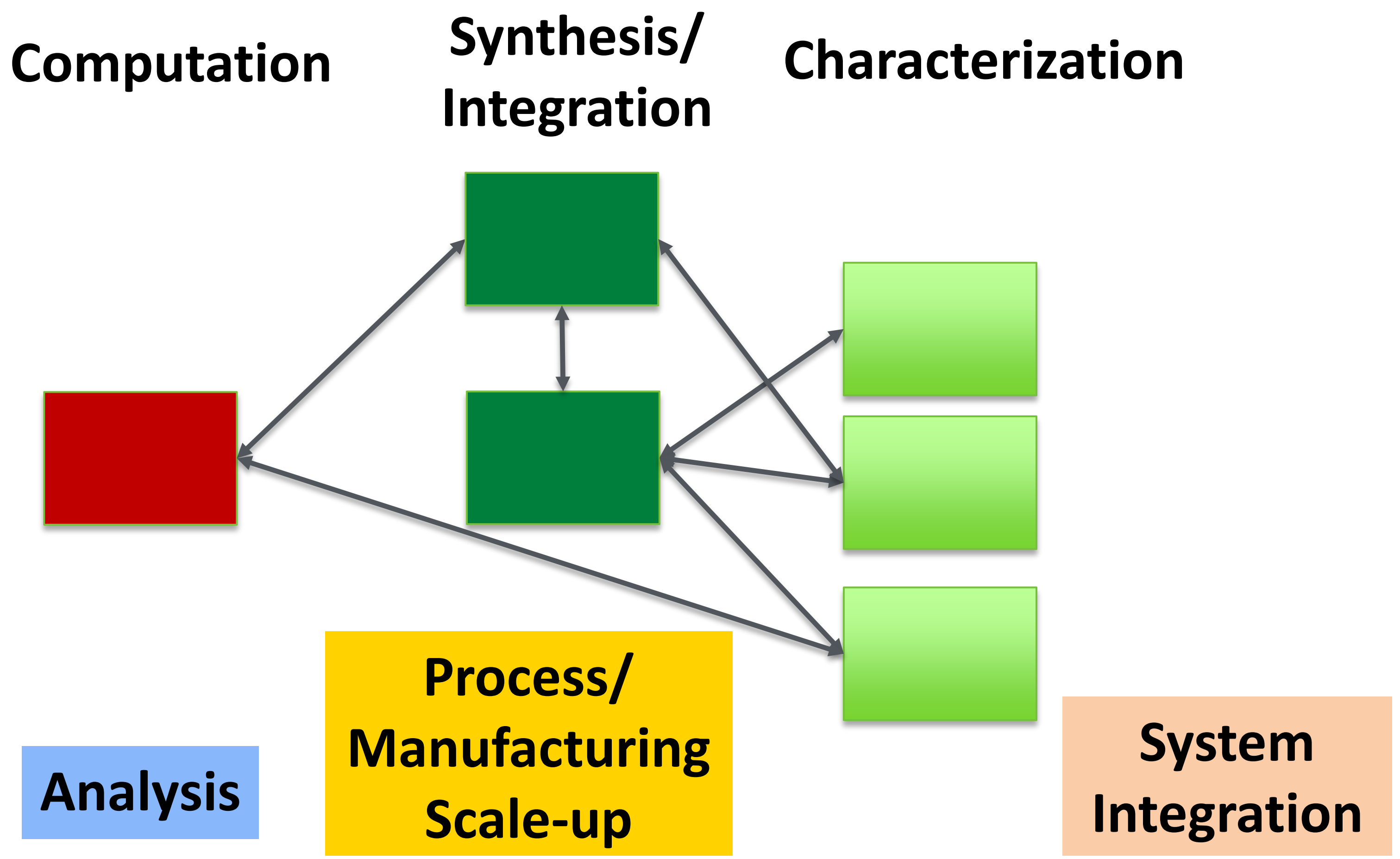
Analysis: 1	**Characterization: 13**
Computation: 5	**Synthesis/Process: 3**
System Integration: 4	**Process/Scale up: 5**

Category 3

Analysis: 0	**Characterization: 2**
Computation: 1	**Synthesis/Process: 1**
System Integration: 0	**Process/Scale up: 1**

- **Nodes** comprise **tool, technique, and expertise** including uniqueness
- Category refers to availability, readiness and relevance to AE and not necessarily the expense and time commitment
- Note that **many nodes span classification areas** (analysis, synthesis, characterization, etc.) **and different technologies** (LTE, HTE, HT)

Node Usage



- Projects can/should use multiple nodes to leverage national laboratory capabilities and progress the project
  - Not all types of nodes have to be used

Computational Tools & Modeling Capabilities

1. DFT and ab initio calculations for water splitting including real-time time-dependent density functional theory (LTE, 2: HTE)
2. Multiscale modeling of water-splitting devices (LTE, 2: HTE)
3. Computational materials diagnostics and optimization of photoelectrochemical devices (LTE)
4. Uncertainty quantification in computational models of physical systems (HTE, LTE)
5. Suite of codes for continuum –scale physics modeling (Albany (1: HTE, LTE), SPPARKS (2: HTE), Peridigm (2: HTE))
6. Suite of codes for atomistic modeling (LAMMPS (1: HTE, LTE), Socorro (2: HTE, LTE))
7. Experimental and computational Materials Data infrastructure (ALL)

1. First principles materials theory for advanced water splitting pathways (HTE, LTE)
2. Ab initio modeling of electrochemical interfaces (LTE)

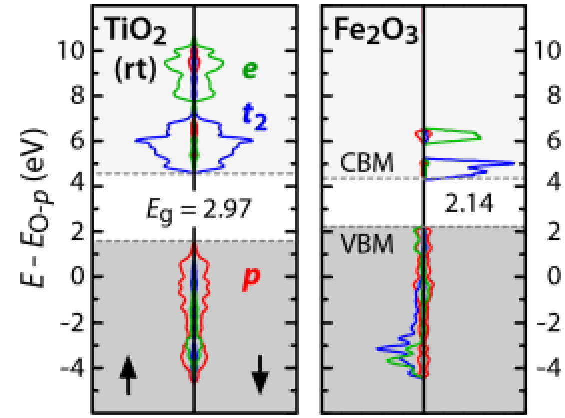
1. Suite of codes for continuum –scale physics modeling (Moab (3: HTE, LTE))

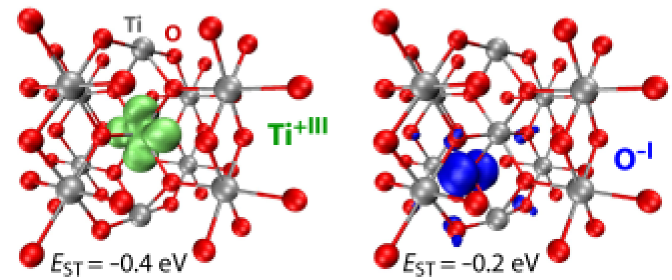
Ab-initio, other, multiphysics

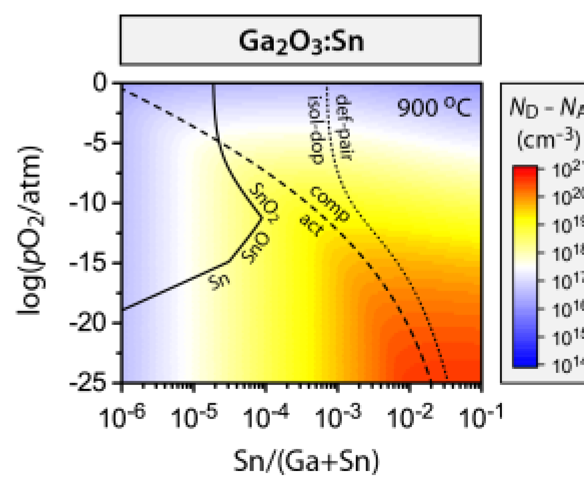
Note that many nodes span different technologies

First Principles Materials Theory for Advanced Water Splitting Pathways (2: HTE, LTE)

- Electronic structure prediction
  - Accurate band gap prediction for semiconductors, including transition metal compounds
  - Band-structure, effective masses, density of states, ionization potential, band offsets, optical properties
- Defects and alloys
  - Defect equilibria from first-principles, including effects due to defect-pair association
  - Small-polaron transport vs band-like transport
  - Alloys: Mixing enthalpy and phase diagrams
  - Ionic diffusion pathways, energy barriers
- Materials Design and Discovery
  - Structure prediction for new compounds
  - Thermodynamic stability range



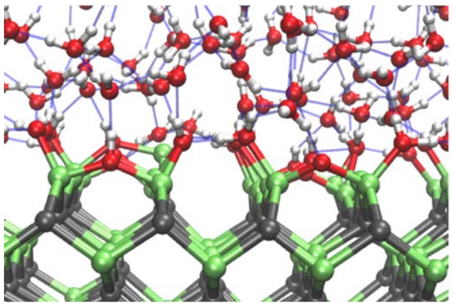




Ab initio modeling of electrochemical interfaces (2: LTE)

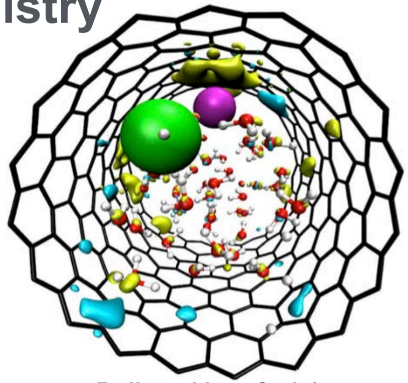
Solid-liquid interfacial chemistry

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



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

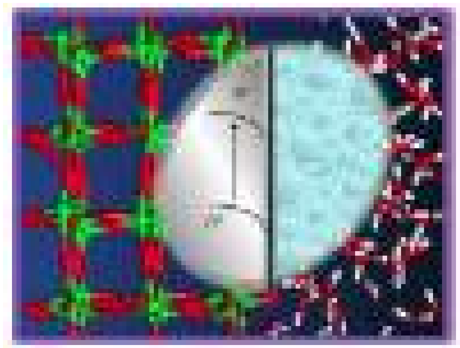
JPCC 120, 7332 (2016)



Bulk and interfacial properties of aqueous electrolytes

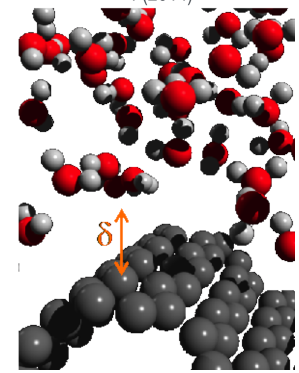
Electronic properties of interfaces

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



Electronic properties of electrode-electrolyte interfaces (from GW)

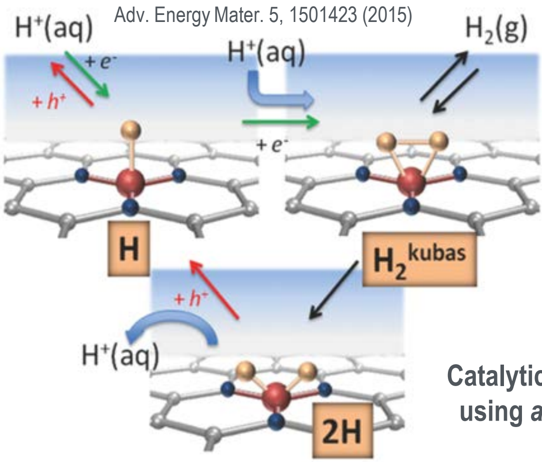
PRB 91, 125415 (2015); JPCC 118, 4 (2014)



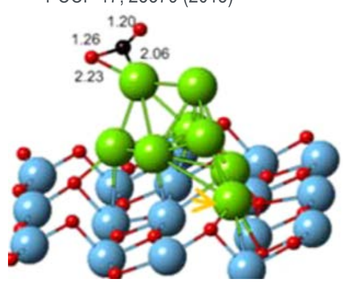
Simulations under applied bias or photobias

Electrocatalysis and photocatalysis

Adv. Energy Mater. 5, 1501423 (2015)

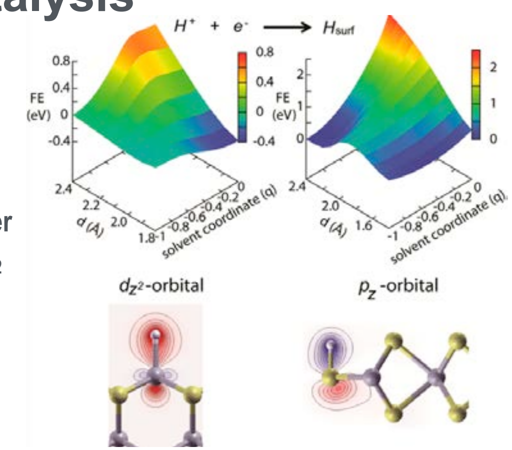


JPCC 118, 26236 (2014); PCCP 17, 25379 (2015)



Catalytic activity predictions using *ab initio* descriptors

Charge-transfer barriers for H_2 evolution

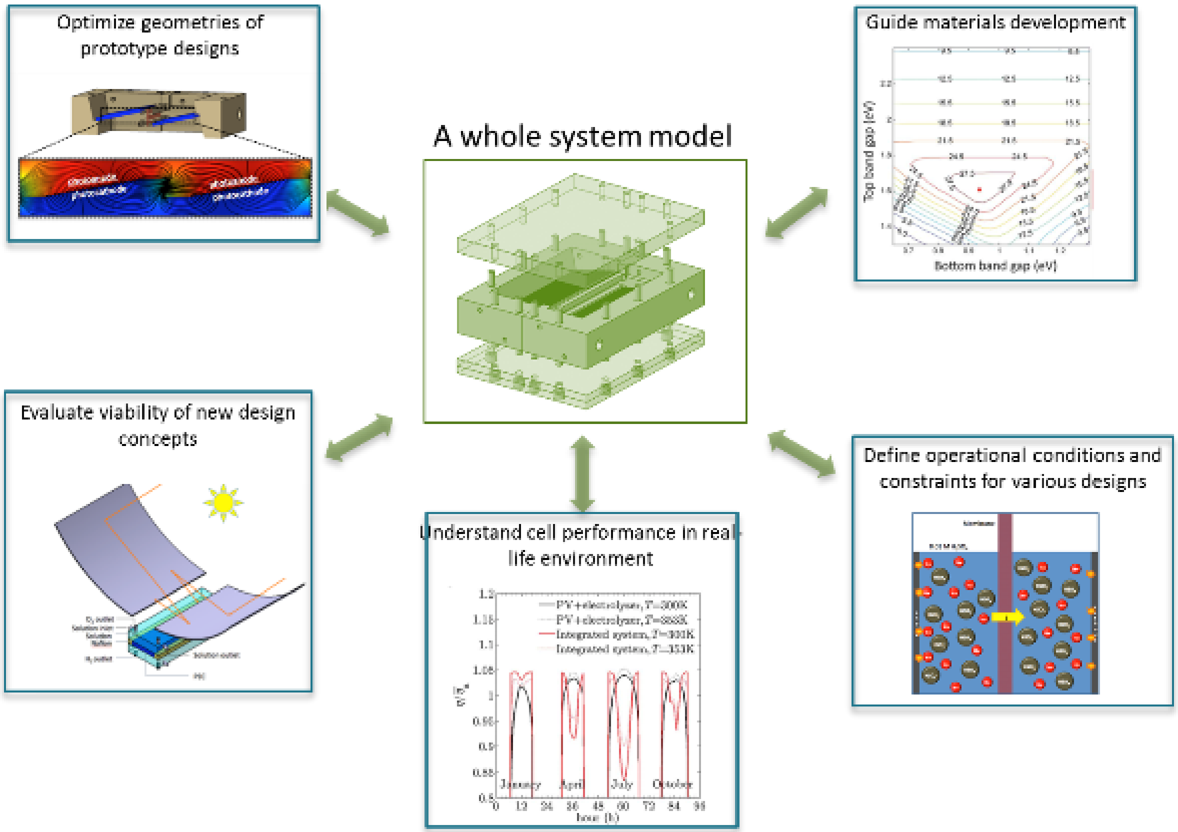


JPCC 117, 21772 (2013)

Multiscale, Multiphysics Modeling (1: LTE, 2: HTE)

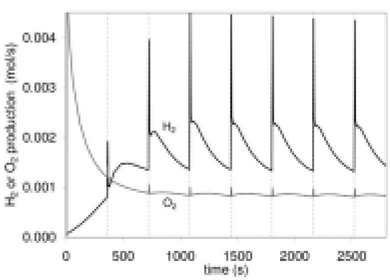
Use continuum multiphysics mathematical modeling to predict and optimize cell performance

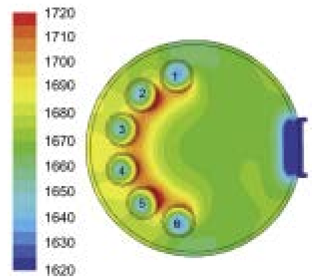
- Extensive experience in modeling electrochemical and water-splitting technologies
  - Models ready to go
  - Help with parameter estimation
  - Sensitivity and optimization studies
- Help develop models for specific materials set and conditions

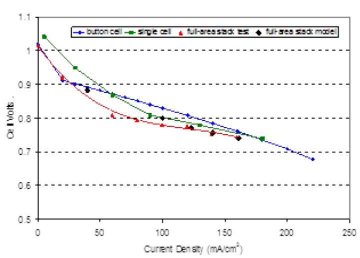


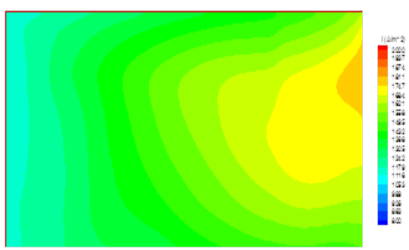
Multi-scale thermochemical and electrochemical modeling for material scale-up to component design (2: LTE)

2









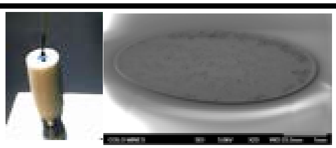
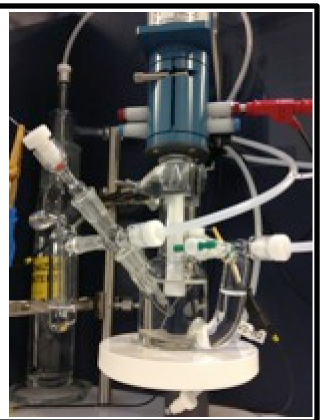
Purpose: This capability develops computational tools to **enable the implementation of materials into a component (cell, stack, or reactor) and to assess their performance, lifetime and reliability through high-fidelity modeling of a component design.**

Key Features:

- NREL component and system modeling expertise can support material integration into the hydrogen generation devices and system configuration.
- The component modeling tools use ANSYS software as a solution framework, by adding fundamental thermochemical, electrochemical, and thermomechanical models in customized user defined functions.
- The modeling practices were previously successfully applied for fuel cell stack design and solar thermochemical hydrogen process (STCH).
- The capability can be used for advanced electrolysis and solar thermochemical hydrogen conversion development as a general tool for electrolyzer design or solar reactor performance optimization.

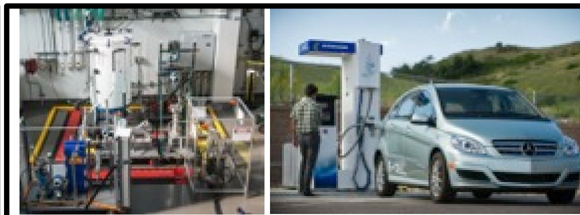
- Martinek, J., Viger, R., Weimer, A.W. (2014) "Transient simulation of a tubular packed bed solar receiver for hydrogen generation via metal oxide thermochemical cycles" Solar Energy 105 pp. 613-631.
- Ma, Z., Venkataraman, R., Farooque, M. (2009). "Modeling", In J. Garche, C. Dyer, P. Moseley, Z. Ogumi, D. Rand and B. Scrosati, editors. Encyclopedia of Electrochemical Power Sources, Vol 2.Amsterdam: Elsevier; 2009. pp. 519–532.

Laboratory Pathway – From Powders to Power

Electrochemical Characterization:
RDE & RRDE stations for Mass & Specific Activity, ECA, ORR; EQCMB, Seiras

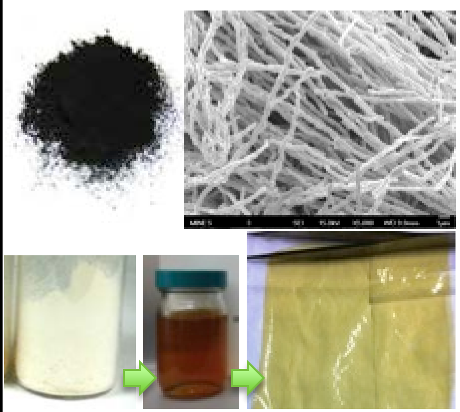
Roll-to-roll manufacturing & Thin Film Quality Control :
Micro-gravure & slot die coating, Development of inspection tools



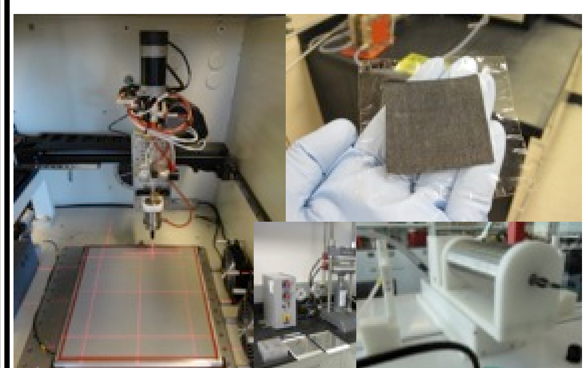
H_2 Generation & Dispensing
Supply for Labs, testing, & fueling
Dispensing at 350 and 700 bar

Powders → Power

Material Synthesis:
Catalyst &
Membrane Development

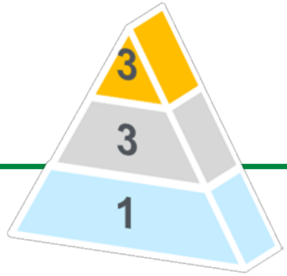


MEA integration
Coating, Spraying, Painting, Electrospinning, Lamination, Hot Press Transfer, Edge protection



Performance Evaluation:
In-situ Diagnostics, PEMFC, AEMFC, Electrolyzer; Single Cell, Stacks, Spatial

Synthesis Capabilities



1. Electrolysis catalyst synthesis, ex-situ characterization, and standardization (LTE)
2. Novel Membrane Fabrication and Development (LTE)
3. Spray pyrolysis (LTE & HTE)

1. High-throughput combinatorial experimental thin films (LTE & HTE)
2. Separators for hydrogen production (LTE & HT)
3. Temporal analysis of Products (TAP) Reactor System (HTE)

1. Novel materials and characterizations for electrocatalysis (LTE & HTE)

Note that many nodes span classification areas and different technologies

Novel Membrane Fabrication and Development for Low Temperature Electrolysis (1: LTE)

NREL leads world class research in the *synthesis and fabrication of polymer electrolyte membranes* and ionomers for electrochemical device applications (PEM and alkaline exchange membrane (AEM) electrolyzers and fuel cells).

Polymer Synthesis

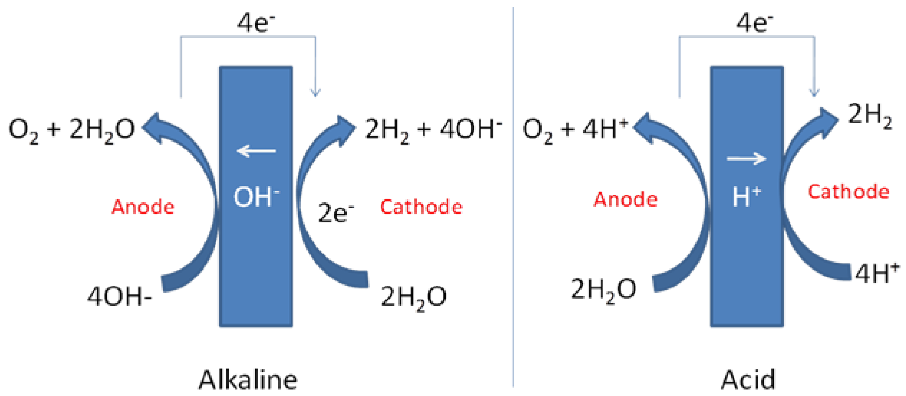
- Synthesis and/or modification of both hydrocarbon and fluorocarbon polymer backbones
- Optimization of tether chemistry
- Development/attachment of novel ion exchange groups
- Characterization of degradation mechanisms and overall stability

Membrane Fabrication

- Synthesized polymers are fabricated into membranes via several techniques, including doctor blade, Meyer rod, hand spread, or roll to roll coating
- Novel morphologies enabled with world-class dual-fiber electrospinner
  - Humidity control between 5 and 80%RH

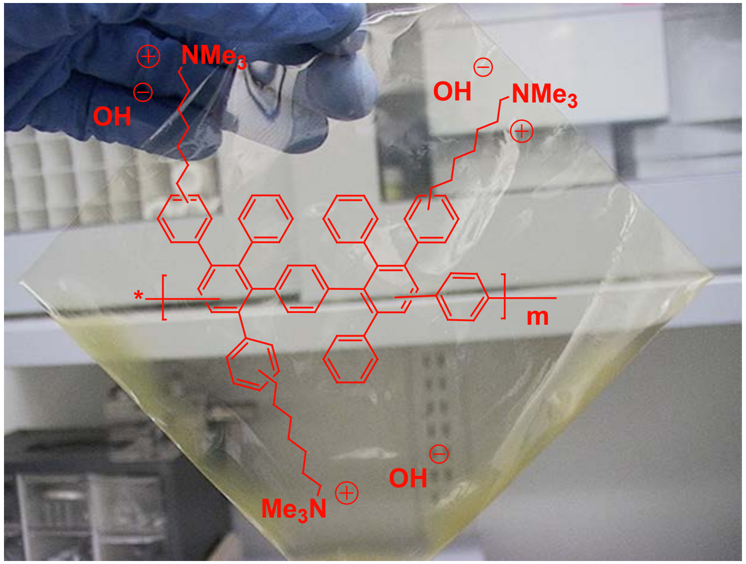
Separators for Hydrogen Production (Sandia Membrane) (2: LTE & HT)

Alkaline vs Acidic Electrolysis



- Non precious metal catalysis
- Low cost separator

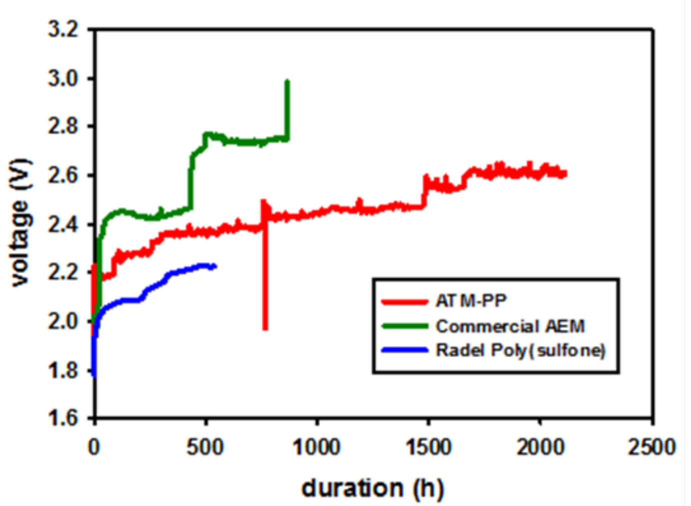
- Precious metal catalysis
- Nafion separator



J. Polym. Sci. B. Polym. Phsy. 51 (2013) 1736-1742

- Alkaline electrolysis reduces precious metal requirements
- Sandia developed advanced anion exchange membrane
- Highly durable under alkaline electrolysis conditions
- Materials highly tunable for application and use

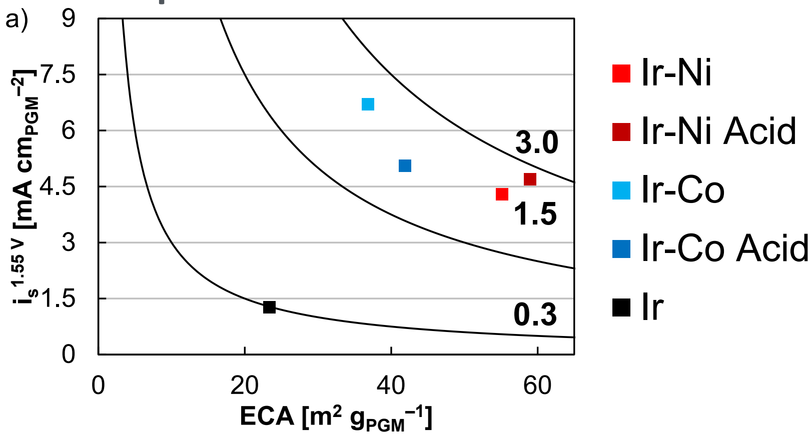
+2000 h Sandia membrane performance



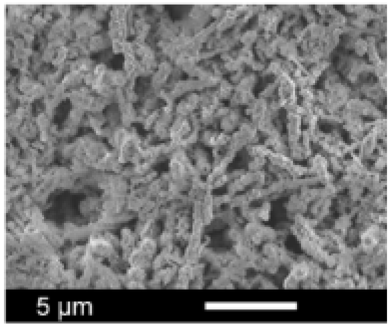
Chem Mater 26, 19 (2014) 5675-5682

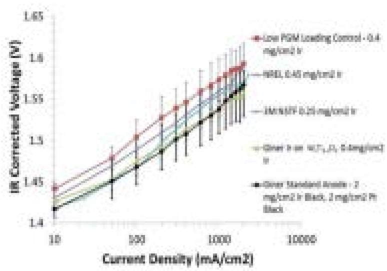
Electrolysis catalyst synthesis, ex-situ characterization, and standardization (1: LTE)

- NREL synthesizes Ir & Pt catalysts for PEM, AEM electrolysis
- 10 times greater activity than nanoparticles

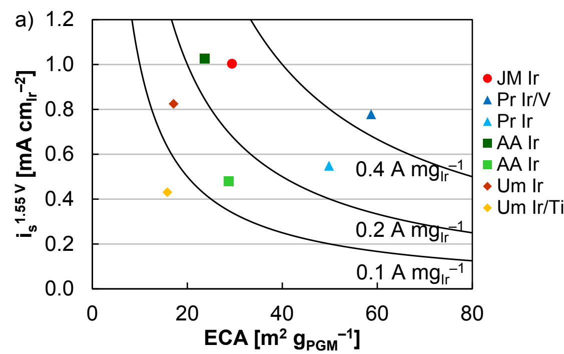


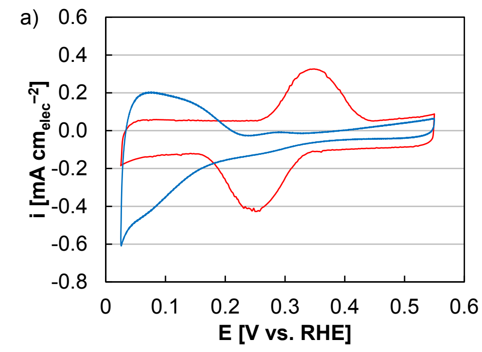
- Fundamental characterization
- Verification with device performance



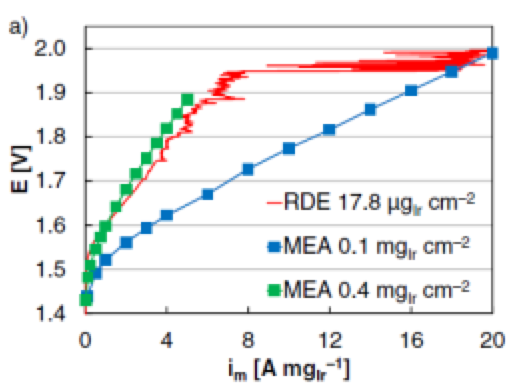


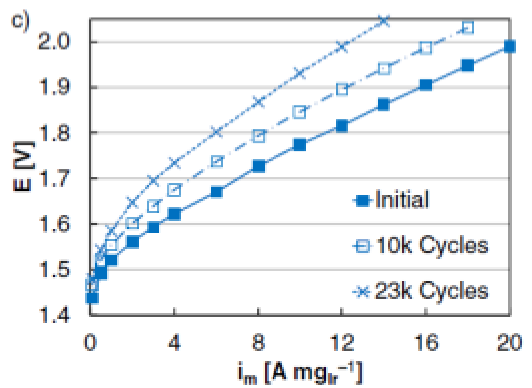
- Baseline catalyst activity
- Surface area measurements on Ir and Ir oxides





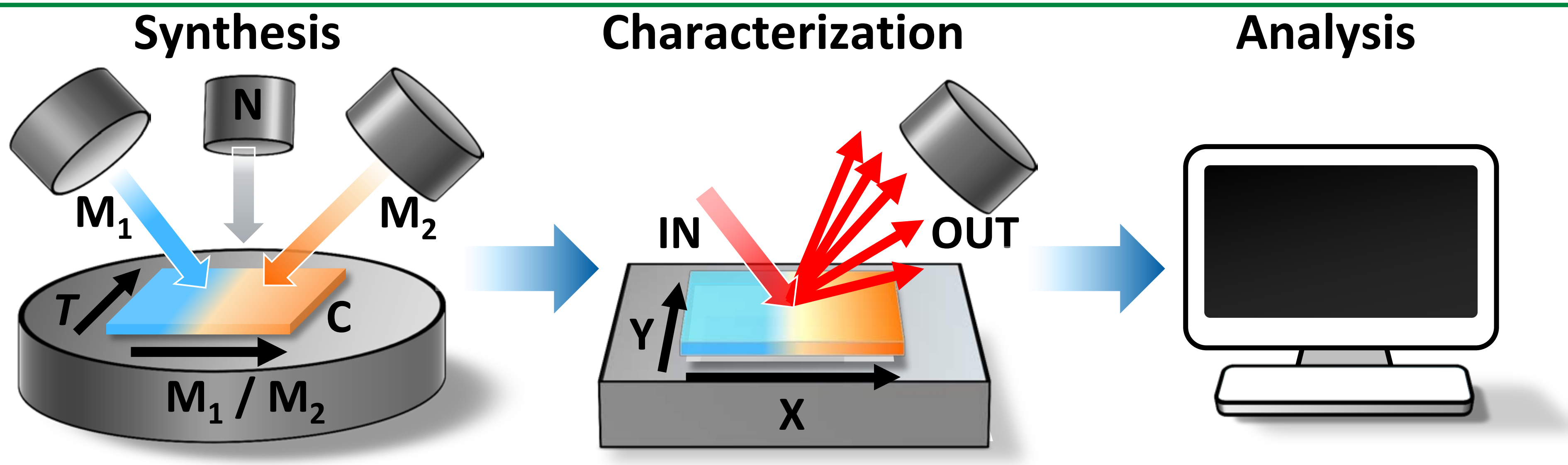
- Correlate ex-situ performance and durability to device





High-Throughput Experimental (HTE) Thin Film Combinatorial Capabilities (2: LTE & HTE)

2



Combinatorial Synthesis
- multi-element thin films of nanoparticles (metals, oxides, nitrides, sulfides)
- gradients (composition, temperature, film thickness, nanoparticle size etc)
- physical vapor deposition techniques (sputtering, pulsed laser deposition)
- substrates (highly oriented pyrolytic graphite, metals, glass etc)

Spatially-resolved characterization
- chemical composition (XRF, RBS)
- crystallographic structure (XRD, Raman)
- microstructure (SEM, AFM)
- surface properties (PES, KP, PYS)
- optical (UV/VIS/FTIR absorption, PL)
- electrical ((photo)conductivity, Seebeck)
- electrochemical (SECM, scanning droplet cell under development)

+ Automated data analysis (Igor PRO, HTE materials database)

Contact: Andriy.Zakutayev@NREL.gov

Process/Manufacturing Scale-Up Capabilities

1. High-throughput approaches to scaling new PEM electrolysis electrodes using relevant production technologies (LTE)

1. Fabrication of Designer Catalytic Electrode at Multiple Length Scales Using Additive Manufacturing (LTE & HTE)
2. Advanced Materials for Water Electrolysis at Elevated Temperatures (HTE)
3. Digital Printing and Coating (LTE)
4. Clean rooms with surface preparation (LTE & HTE)
5. Photoelectrochemical device fabrication facility (LTE)

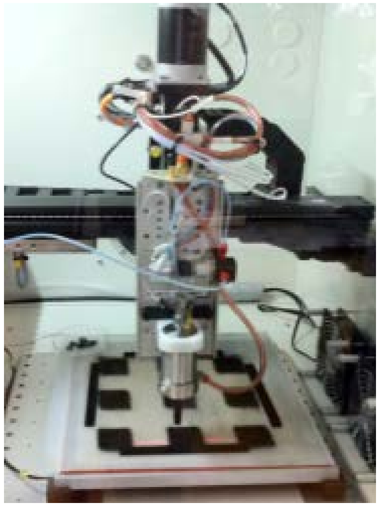
1. Metal-supported SOEC cell (HTE)

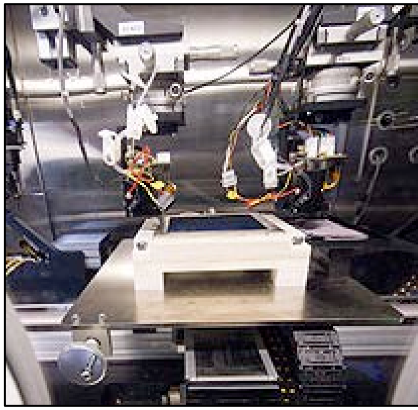
Note that many capabilities span different classification areas, technologies and techniques

High-throughput approaches to scaling PEM electrolysis electrodes using relevant production technologies (1: LTE)

High-throughput (HT) 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

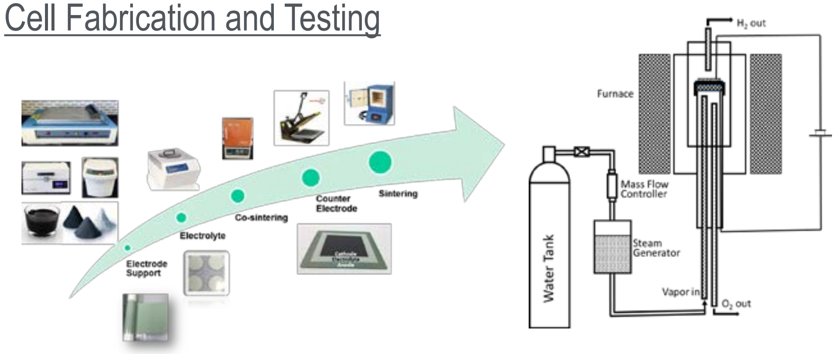
- Small-scale ink processing
  Formulation, mixing, viscosity, rheometry
- Small-scale coating
  Spin, knife, rod
- Spray coating
  Ultrasonic, aerosol jet, ink jet, electro-spin/spray
- R2R coating
  Slot die, micro-gravure

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

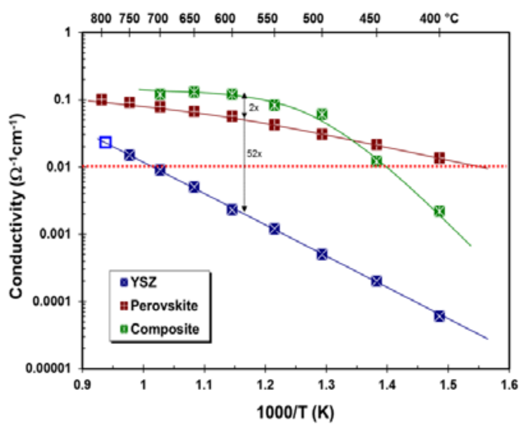
Advanced Materials for Water Electrolysis at Elevated Temperatures (2: HTE)

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

Characterization Capabilities

1. Surface Analysis Cluster Tool (LTE, HTE)
2. Scanning droplet cell for high-throughput electrochemical evaluation (LTE)
3. Ex situ spatial characterization capabilities to support cell component integration and scaling studies (LTE, 3: HTE)
4. In-situ and operando nanoscale characterization capabilities for photoelectrochemical materials and integrated assemblies (LTE)
5. Electron beam and in-situ photon beam characterization of PEC materials and Devices (LTE)
6. In-situ/Operando X-ray characterization of electronic structure in photoabsorber materials (LTE)
7. Corrosion analysis of materials (LTE, 3: HTE)
8. Probing and mitigating chemical and photochemical corrosion of electrochemical and photoelectrochemical assemblies (LTE)
9. Characterizing degradation processes at photoelectrochemically driven interfaces (LTE)
10. Contamination related capabilities (LTE, 3: HTE)
11. SIMS (LTE, HTE)
12. Photophysical characterization of photoelectrochemical materials and assemblies (LTE)
13. Analysis and characterization of hydrided material performance (HTE)

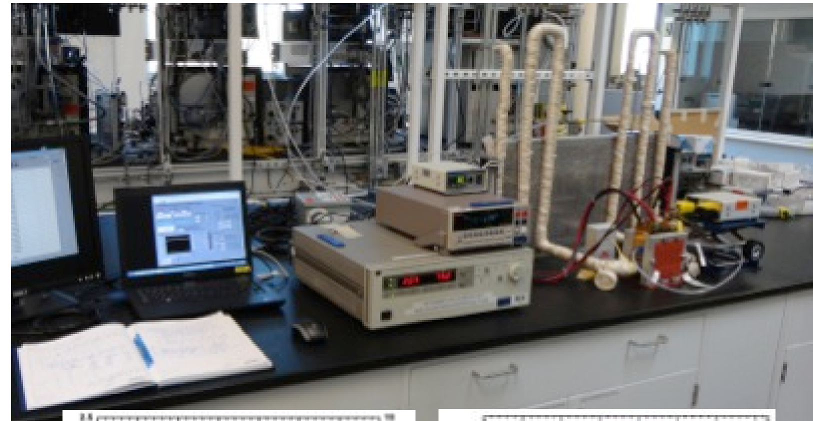
1. In-situ Testing Capabilities for Hydrogen Generation (1 kW – 250 kW) (LTE)
2. Electrochemical and durability performance evaluation of high temperature electrolysis cells and stacks (HTE)
3. Photoelectrochemical device in-situ and operando testing using x-rays (LTE, HTE)
4. Advanced electron microscopy (LTE, HTE)
5. High-Temperature XRD and Complementary Thermal Analysis (HTE)
6. Water-splitting device testing (LTE)
7. Ionomer Characterization and Understanding (LTE)
8. Characterization of high temperature catalyst and electrolyzer components for hydrogen production (HT)
9. Controlled environment, elevated temperature test suite (HTE)

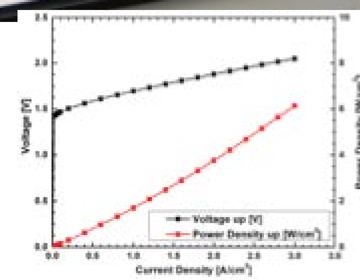
1. Near-ambient electrochemical XPS (LTE, HTE)
2. High-temperature corrosion, corrosion mitigation, and materials durability improvement for hydrogen production (HT, HTE)

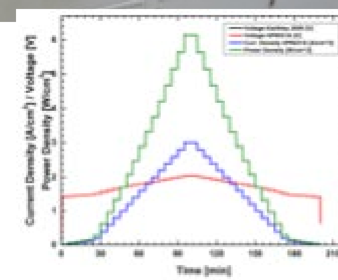
Note that many capabilities span different classification areas, technologies and techniques

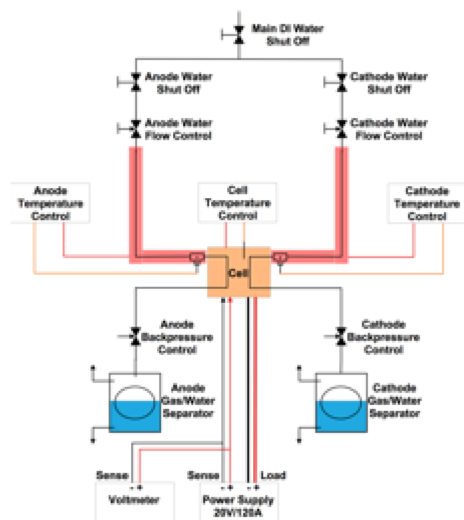
In-situ Testing Capabilities for Hydrogen Generation (1 kW – 250 kW) (1: LTE)

- 3x test systems with variety of capabilities
- Equipment benchmarked with leading research institutions & industry
- Operation of stacks and system components up to at least 250 kW
- Operation of single cells and small stacks up to 12.5V/250A
    - Up to 50 bar H_2 pressure
    - AC impedance
    - Anode & cathode product gas analyzer
- H_2 pump option with hydrogen inlet humidification
    - Up to 5 bar inlet pressure
    - Up to 50 bar outlet pressure

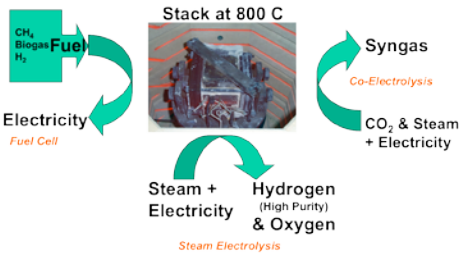




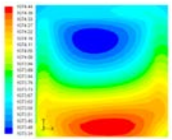




Electrochemical & Durability Performance Evaluation of Solid Oxide Cells & Stacks (1: HTE)



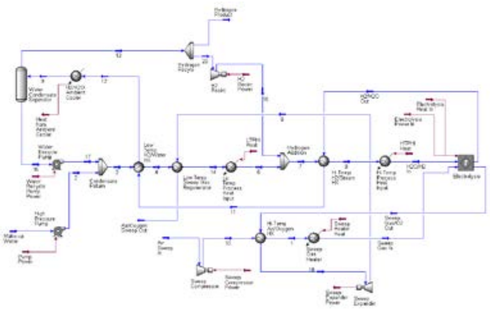
INL can test all operation modes of solid oxide stacks



INL 3D CFD Modeling of Cells and Stacks

INL Pressurized Test Stand

INL 15kW Test Stand



INL 15kW Process Modeling

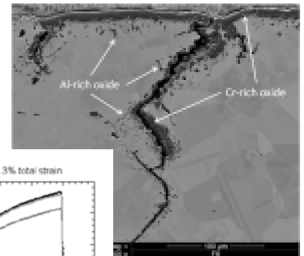
Purpose: This node tests high temperature electrolyzer designs and BOP materials, with post-test examination, to understand materials performance degradation issues.

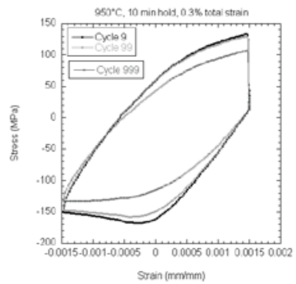
INL's Key Features:

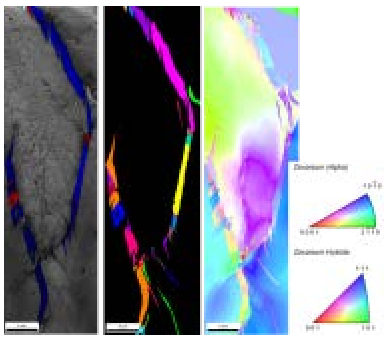
- DOE's lead lab for high T electrolysis under Nuclear Hydrogen Initiative
- World class solid oxide electrolyzer test capabilities
  - Button cells to multi-kW testing of large stack configurations
  - Seven independent test stands, including high pressure stack
  - Reversible, automated, multi-mode, long duration testing
- Significant solid oxide electrolyzer post test examination capabilities
  - SEM/EDS, Auger electron spectroscopy
  - Glow Discharge Atomic Emission Spectrometer
  - 3D Laser Surface Profilometry
  - Computerized Tomography
  - Local Electrode Atom Probe Microscopy
  - Positron Annihilation Spectroscopy
- Advanced analytical methods
  - Atomistic modeling, CFD, and process modeling
- Corrosion testing up to 1100 C in He, H_2, CO, or CO_2 reducing (wet or dry) and/or air, O_2, N_2 He oxidizing environments

Controlled Environment Effects Laboratory (1: HTE)

Microstructure Evolution and Mechanical Property Characterization

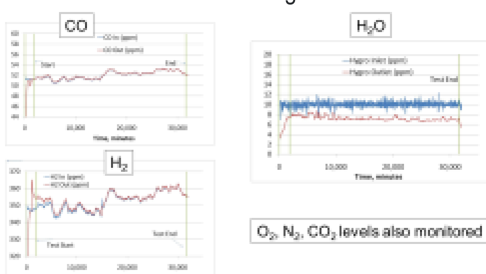






Electron Backscattering Diffraction of Hydrides in Zr

Continuous Monitoring of Environment



Purpose: This node enables controlled environment exposures of alloys in a variety of static and dynamic conditions in order to establish a basis for fundamental materials behavior

INL's Key Features:

- Enables prescreening of candidate alloys that will be exposed to harsh environments at elevated temperatures (hydrogen production/storage)
- Static exposures in controlled environments
  - *Hydrogen atmospheres*
  - *Elevated temperatures*
  - *Helium-rich with low partial pressures of H_2O*
- Mechanical testing in controlled environments
  - *Crack growth, fatigue/creep-fatigue, uniaxial loading*
- Microstructural analysis of test specimens exposed or tested in specialized environments
  - *EBSD analysis of alloys highly dependent upon specimen surface quality*
- Establishment of fundamental mechanisms for input to Multiphysics Object-Oriented Simulation Environment (MOOSE)
  - *Mesoscale behavioral response and microstructural evolution*

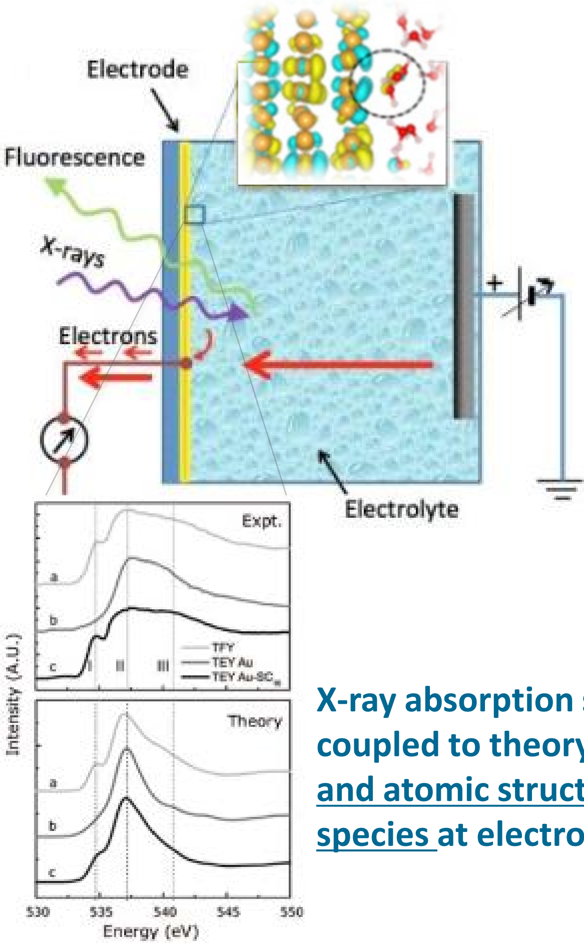
INL Hydriding Furnace

INL Specialized Environment Static Test Chamber

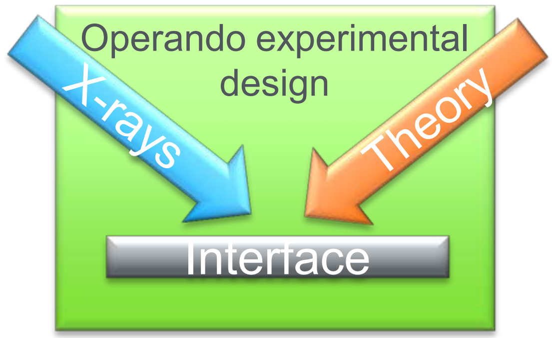
INL Controlled Environment Servo-hydraulic Frame

X-ray Approaches for Understanding (photo)electrochemistry at Interfaces (1: LTE, HTE)

Operando XAS

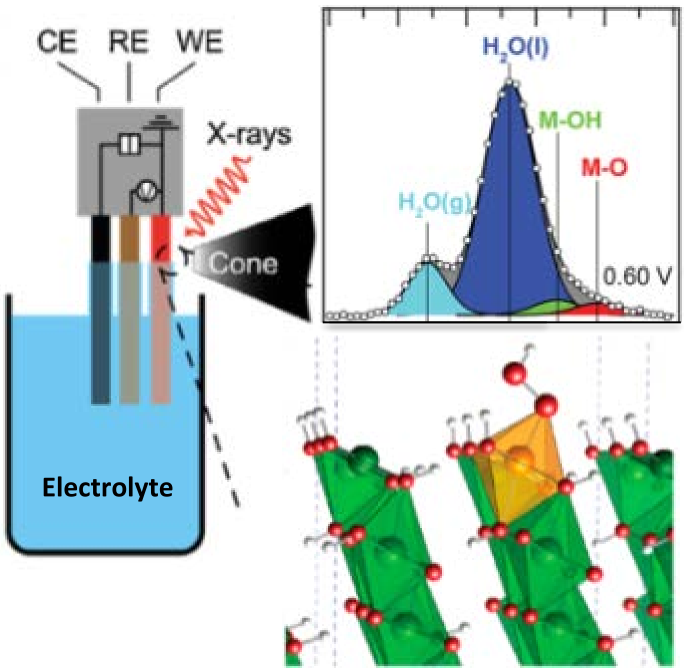


X-ray absorption spectroscopy, coupled to theory, reveals electronic and atomic structure of chemical species at electrode interface



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

Operando ambient pressure XPS

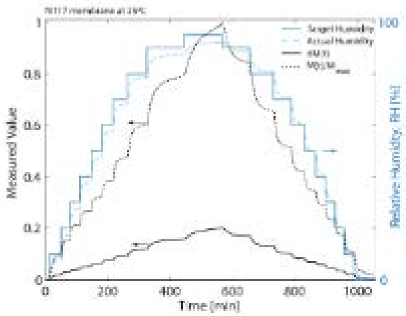


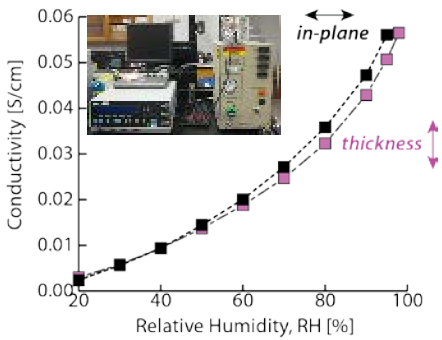
X-ray photoelectron spectroscopy and molecular simulations reveal atomic concentration, chemical speciation, and potential profile at electrode interface

Ionomer characterization and understanding (1: LTE)

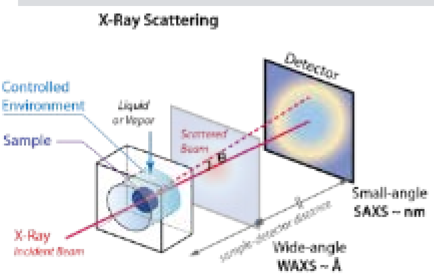
- **Characterization Tools for ionomers,** (ion-conductive polymers) that are used for water splitting

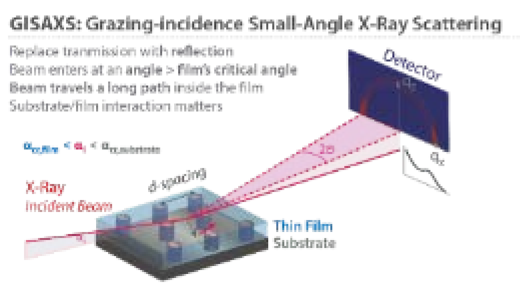
Water uptake/diffusion | ionic conductivity





Structural characterization using X-ray scattering





LBNL capabilities include:

- **thin-film fabrication**

  spin casting, spray coating with a SONO-TEK Exacta Coat System)

- **Property characterization**

  Thin Films: QCM and ellipsometry with RH /T control, profilometry, mechanical properties

  Membranes: macroscale solvent uptake (dynamic vapor sorption), mechanical properties (DMA, Instron), titration, gas permeation (both single gas and mixtures, and dry/wet), density, conductivity and other transport properties in and through the plane as a function of solvent content

- **Structural characterization**

  SAXS/WAXS and GISAXS (for thin films) cells and setups including heating, dry/wet imaging and mechanical testing setup for use in-line at a synchrotron. Also, various equipment to probe the formation of polymers and films including digital light scanning, rheometry, zeta potential.

In accordance with the equipment, there is the associated expertise of using the equipment and analyzing the data

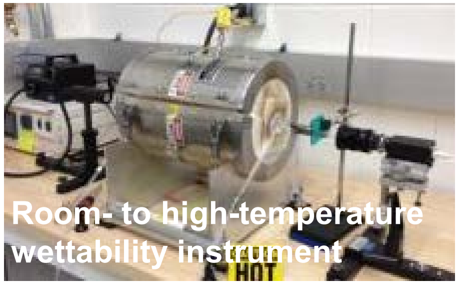
Characterization of Electrolyzer Components for Hydrogen Production (1: HT)

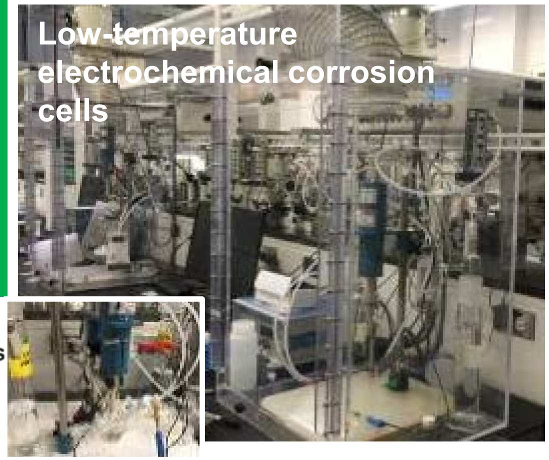
Allows testing components (catalyst and membrane) and membrane electrode assembly collective properties for non-conventional electrolysis

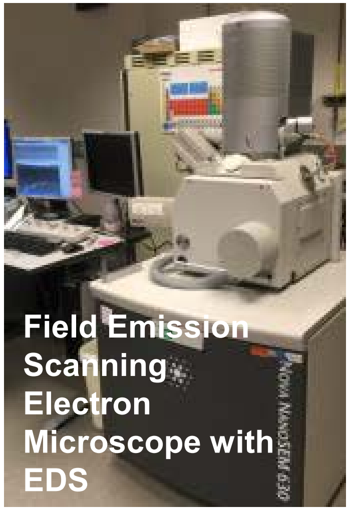
- Catalyst test station-Ex-situ kinetic study of supported catalysts and physical vapor deposited materials on substrates
- Membrane test station-Electrochemical measurement of reactant crossover
- Pressurized Button Cell Test Facility-designed to withstand operation with highly corrosive fluids and at elevated temperatures (130° C) and pressures (150 psia).

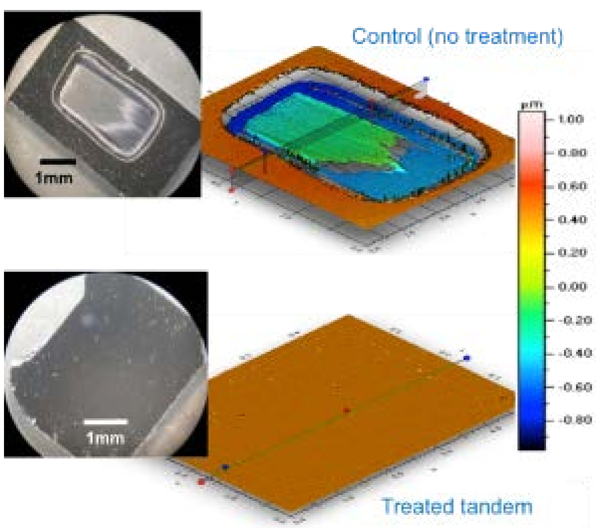
Corrosion analysis of materials (2: LTE, 3: HTE)

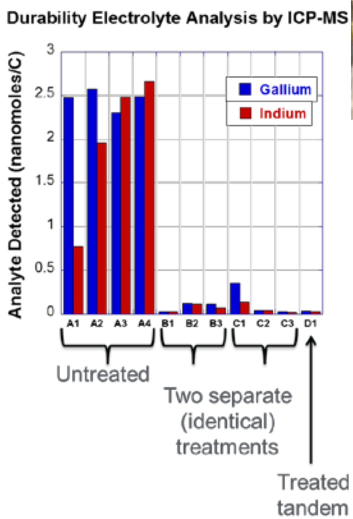
- Electrochemical corrosion and long-term immersion weight-change evaluations at low- and high- temperature in controlled environments
- Strict protocols followed for sample handling
- Characterization before and after degradation for microstructure, chemical and physico-chemical evaluations
- Durability testing and post-mortem optical profilometry

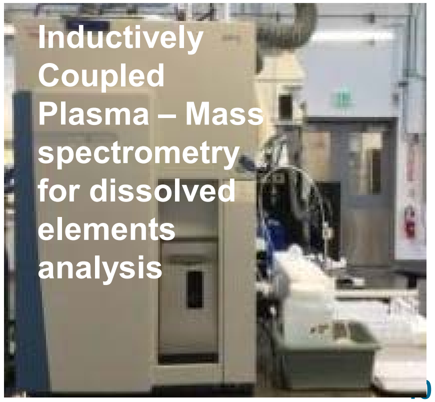










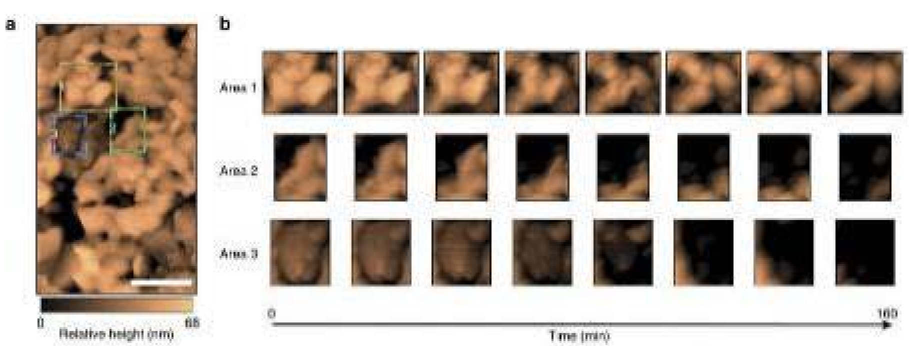


Probing and Mitigating chemical and photochemical corrosion of electrochemical and photoelectrochemical assemblies (2: LTE)

Assessment of the chemical and photochemical stabilities of (photo)electrochemical assemblies

This suite of characterization techniques and expertise comprise:

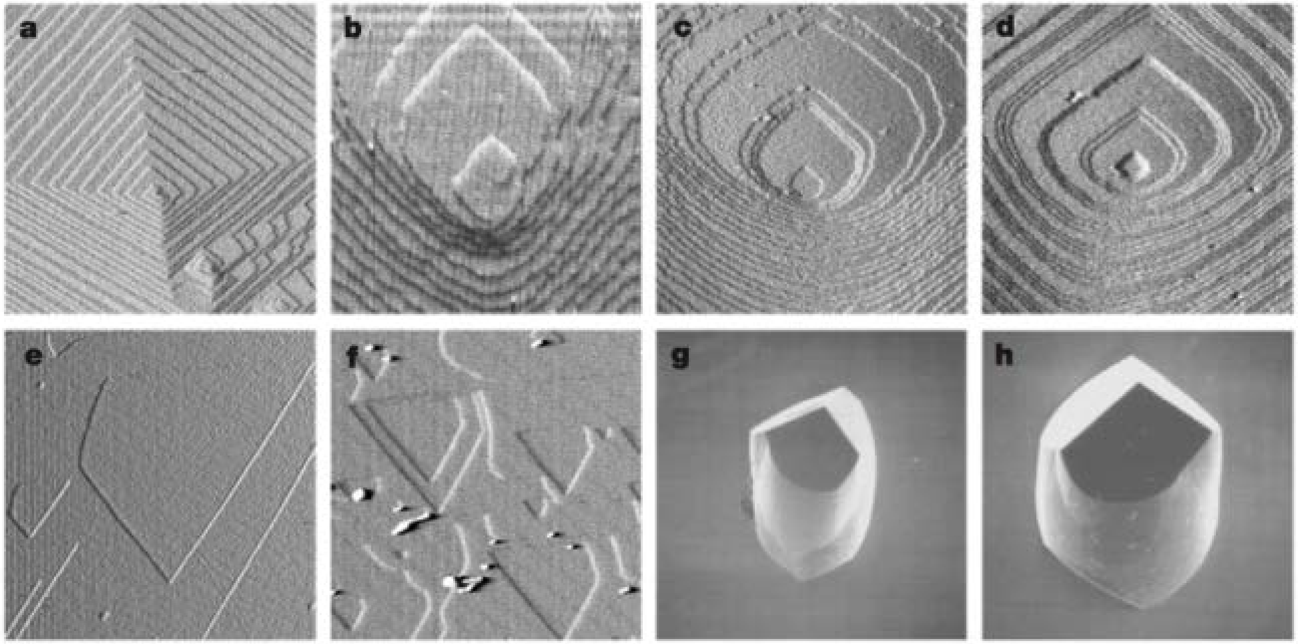
- Electrochemical (EC) and photoelectrochemical (PEC) measurements,
- Inductively coupled plasma mass spectrometry (ICP-MS),
- Electrochemical atomic force microscopy (EC-AFM)



a) EC-AFM scan of $BiVO_4$. b) The three regions indicated in a) were used to monitor corrosion-induced changes to $BiVO_4$ morphology at 20 min increments in 1 M KPi (pH 12.3).

- The specific combination of all these characterization techniques and possible mitigation solutions offers a thorough and complete analysis of electrocatalytic and photoelectrocatalytic materials properties in their working environment
- These analyses are performed on the (photo)electrodes and on the electrolyte utilized to test the performance of the material, with a focus on **material degradation**
- Once identified, various **protection schemes** have been developed that can be used to easily protect the underlying substrates for PEC assemblies

Characterization & Mitigation of Corrosion During Photoelectrochemical Hydrogen Production (2: LTE)



Example: Effect of additive molecules (amino acid) in solvent on mineral (calcite) crystal growth studied with in-situ AFM (a-f) and SEM (g-h)

Orme et al., Nature **411**, 775 (2001); Qiu and Orme, Chem. Rev. **108**, 4784 (2008)

Provide information using a suites of experimental tools (AFM, SPM, SECM, Raman, IR):

- **change of surface morphology induced by relevant factors (potential, pH etc)**
- **identify chemical activities**
- **identify corrosion mechanisms**

and assist developing a corrosion mitigation strategy

Ex situ spatial characterization capabilities to support cell component integration and scaling studies (2: LTE)

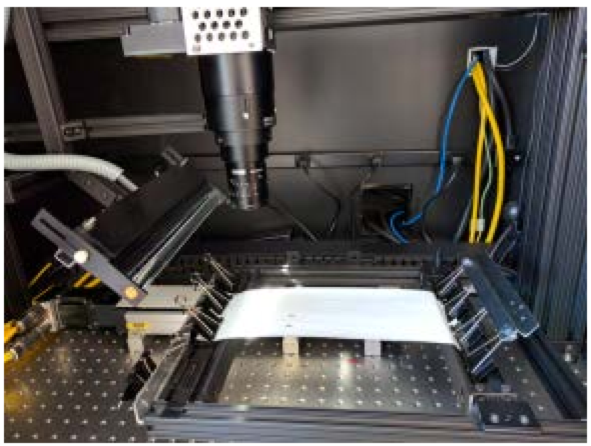
2

Spatial Characterization Concepts

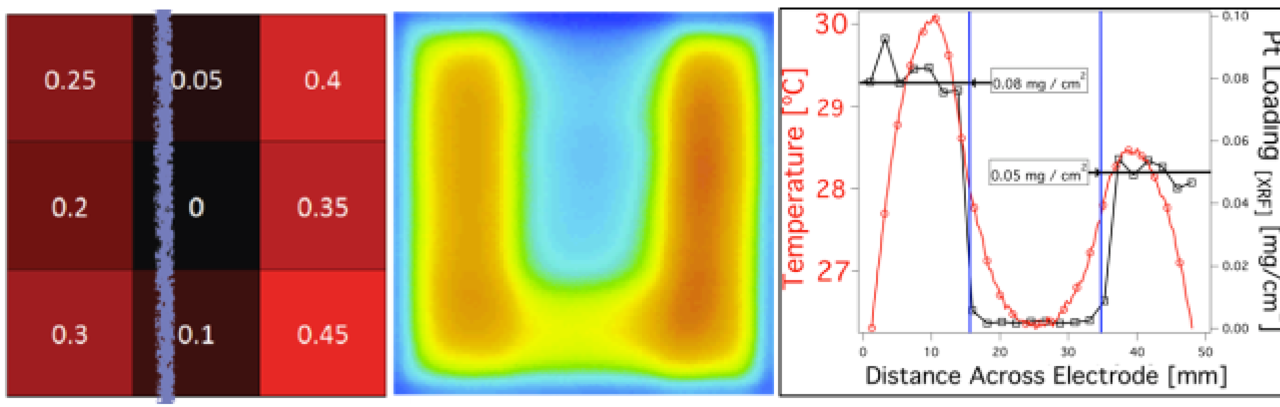
- Active layer mapping of composition, structure, and surface properties
- Real-time imaging of process-related defects
- High-throughput characterization of materials fabricated via combinatorial methods
- Synergistic with high-throughput/scalable processing approaches

Characterization testbeds

- Optical imaging
- Infrared thermography with active excitation
- Mapping XRF
  - Standard system
  - Inert atmosphere system enabling measurement of lower atomic number materials



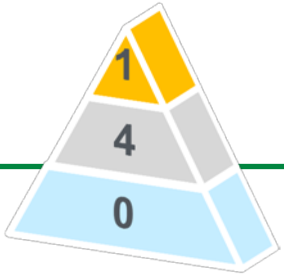
Optical reflectance mapping testbed



Example thermal imaging and mapping XRF of matrixed electrode structure

Enable accelerated mapping of composition and properties of cell materials to assist in the study of optimal uniformity, performance and durability

System Integration



1. Hydrogen Production, Compression, Storage and Utilization - Systems Integration & Infrastructure (LTE)

1. National Solar Thermal Test Facility (HTE)
2. High Flux Solar Furnace (HTE)
3. Engineering of Balance of Plant for High-Temperature Systems (HTE)
4. Concentrating Solar Power Furnace (HTE)

Note that many capabilities span different classification areas, technologies and techniques

Hydrogen Production, Compression, Storage and Utilization - Systems Integration & Infrastructure (1: LTE)

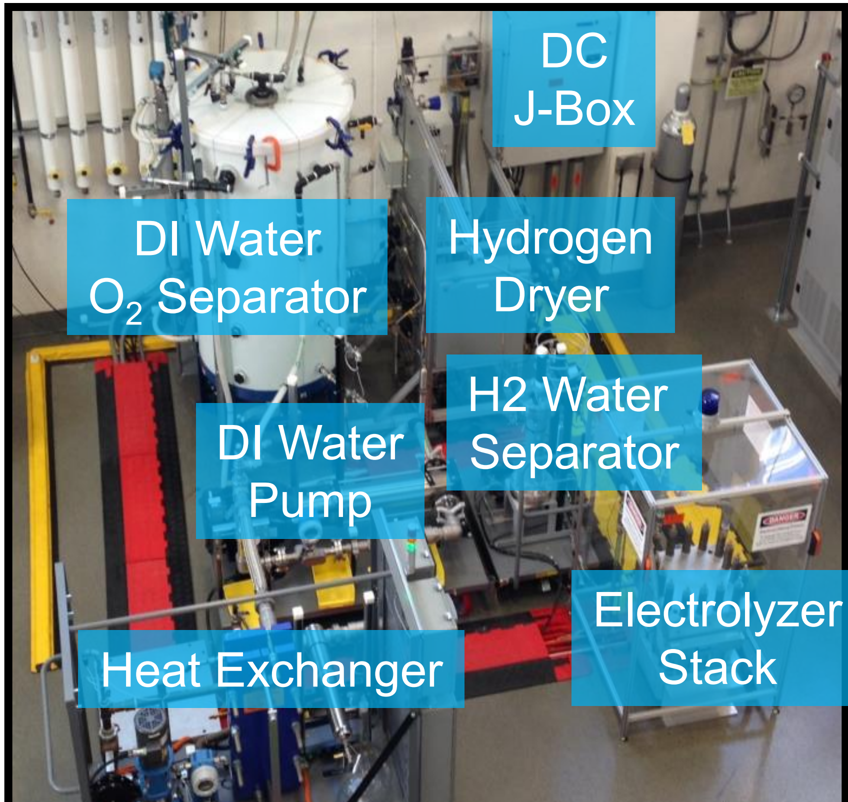
H_2 Generation & Dispensing
Supply for Labs, testing, & fueling
Dispensing at 350 and 700 bar

Located at NREL's Energy System Integration Laboratory

- Flexible platform which enables bread board approach for large active area stack testing
- Large active area stack testing with three 150 kW PEM ad 250 kW stacks demonstrated; 500 kW underway
- AC-DC power supplies with 4,000 ADC and 250 VDC
- Capable of collecting individual cell voltages at different current and stack pressure levels
- Supplies house H_2 and FC car fueling station

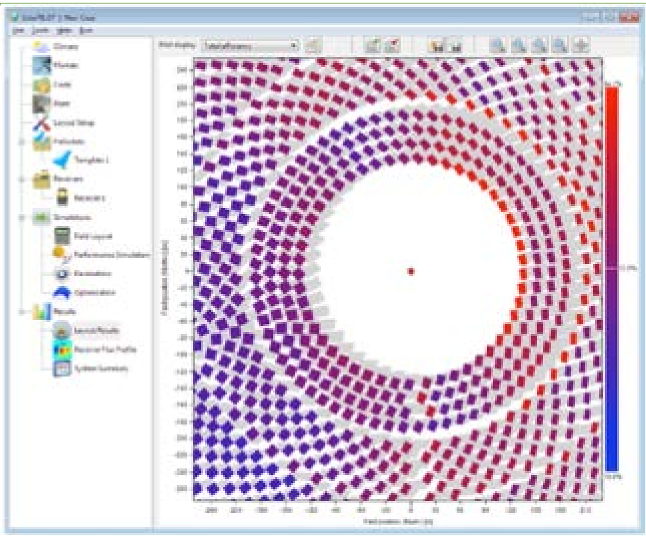
System efficiency improvements in electrolyzer balance of plant

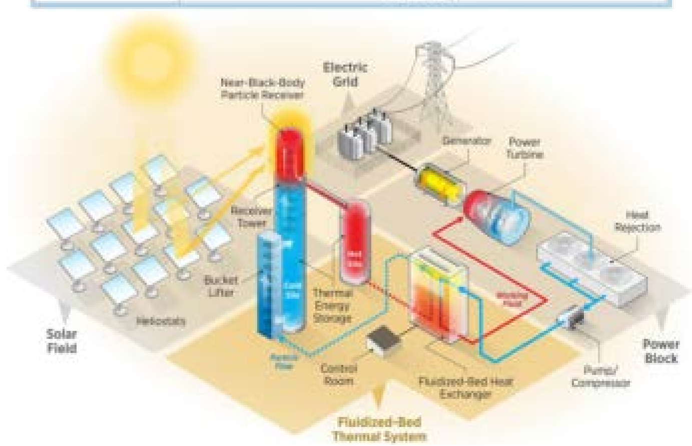
- Drying losses in variable operation with NREL's variable flow drying technique
- Optimize balance of plant based on variable stack power



NREL Electrolyzer Stack Test Bed

Engineering of Balance of Plant (BOP) for high-temperature systems (2: HTE)





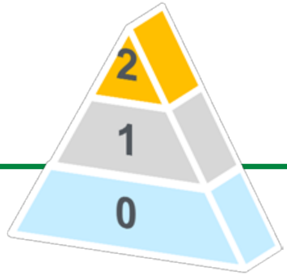
<u>Purpose:</u> This node serves the renewable integration of water splitting materials with engineering design of BOP for high-temperature electrolysis or STCH process.

<u>Key Features</u>:

- NREL uses an integrated suite of solar field, receiver, and thermal storage design tools (SolarPILOT, SolTrace, Aspen, ANSYS Fluent) to maximize the performance of solar thermal and electricity generation.
- Based on the high-temperature water-splitting energy need, the BOP design can provide concentrating solar heat for a wide temperature range.
- The node assists material application through system design for high-temperature electrolysis processes such as solid oxide electrolytic cell (SOEC) and hybrid solar thermochemical hydrogen (STCH) production.
- Leveraging projects funded through the DOE SETO SunShot Program, NREL’s solar development has a unique portfolio of integrated capabilities dedicated to supporting the design of solar-thermal BOP components and systems.

- Zhiwen Ma, Methods and Systems for Concentrated Solar Power, U.S. Patent No. 9,347,690 B2, May 24, 2016.
- Janna Martinek, Zhiwen Ma, “Granular Flow and Heat Transfer Study in a Near-Blackbody Enclosed Particle Receiver,” doi: 10.1115/1.4030970, J. Sol. Energy Eng. 2015; 137(5):051008-051008-9.

Analysis Capabilities



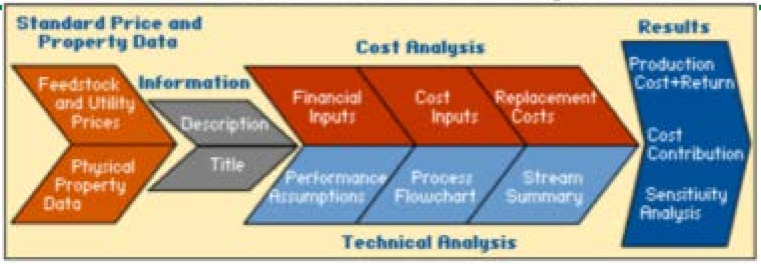
1. Technoeconmic analysis (TEA) of hydrogen production (ALL)
2. Advanced water-splitting materials requirements using flowsheet development and technoeconomic analysis (HT, HTE)

1. Prospective LCA model for 1-GW scale PEC hydrogen plant (LTE, HTE)

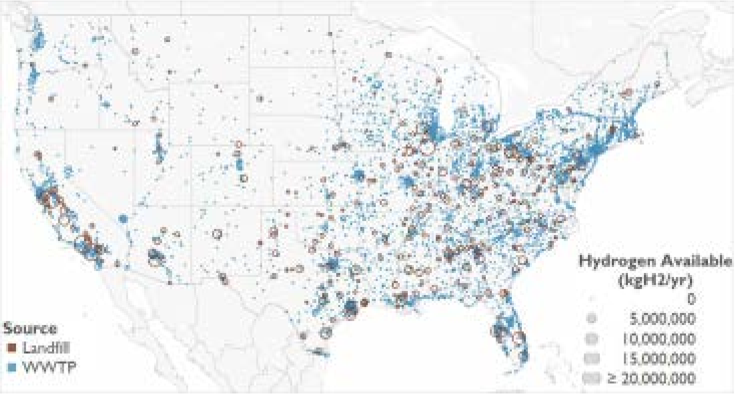
Note that most, if not all projects, will utilize these nodes

Technoeconmic analysis (TEA) of hydrogen production

H2A Production Cash Flow Analysis Tool

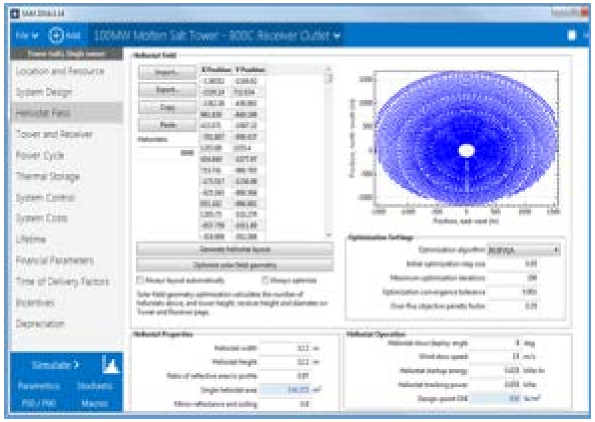


- Hydrogen Analysis (H2A) models
  - Production, Delivery, and Fuel Cells
  - Discounted cash flow framework
  - Models are transparent and public
    http://www.hydrogen.energy.gov/h2a_analysis.html



- Scenario Evaluation and Regionalization Analysis (SERA)
  - Optimizes least cost spatial-temporal infrastructure in response to hydrogen demand
  - Optimization across all pathway options
  - Sub-models explore finance options

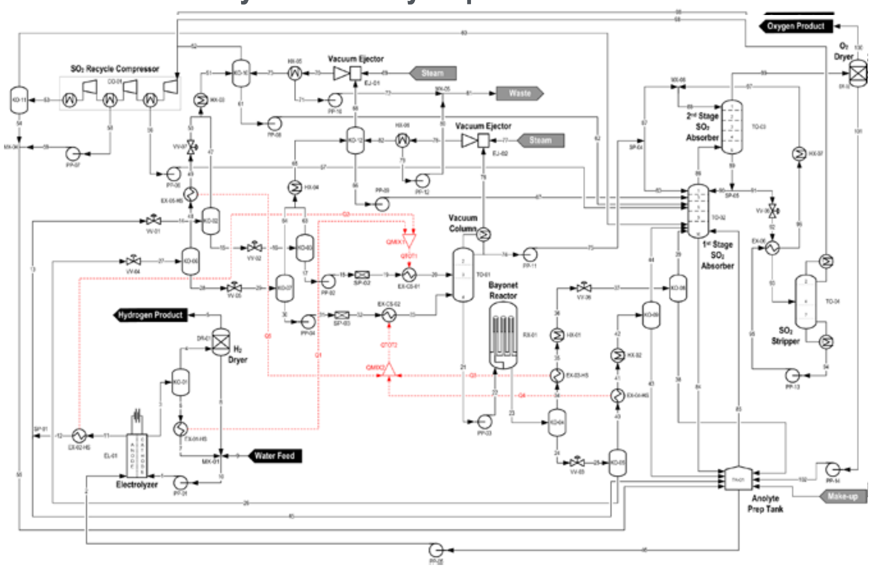
- NREL System Advisory Model (SAM)
  - Renewable resources including solar, wind, geothermal.
  - Economic and generation capacity models for planning
  - https://sam.nrel.gov/



- Hydrogen Financial Analysis Scenario Tool (H2FAST)
  - Standard financial accounting framework for H2A cost analysis models
  - Inform investment decisions by providing end users a tool to explore the financial aspects of station installations
  - Three ways to use H2FAST: Web, Spreadsheet, Business case scenario tool (BCS)

Advanced Water-Splitting Materials Requirements Based on Flowsheet Development and Techno-economic Analysis (TEA) (1: HT, HTE; 3: LTE)

Hybrid sulfur cycle process model

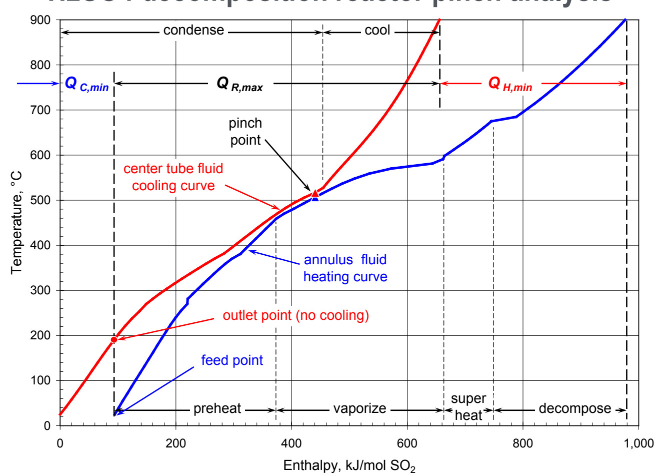


Unique capability for high-temperature water-splitting process development, modeling, and simulation

- To define materials performance requirements
- To identify process stream conditions
- To determine potential impacts of materials improvements on process performance
- To quantify economic impacts and H_2 production cost using H2A

Extensive experience with nuclear and solar heat source designs

H2SO4 decomposition reactor pinch analysis



Use widely accepted commercial off-the-shelf (COTS) modeling tools customized as needed

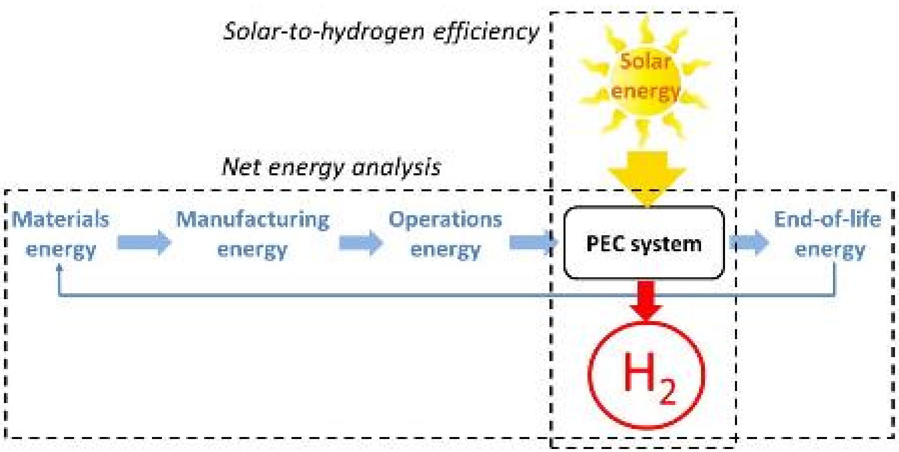
- To build and validate complex electrolyte properties models for thermochemical cycles
- To model individual flowsheet components at any appropriate level of detail
- To optimize overall process energy and resource utilization
- To generate credible capital and operating costs
- Using H2A for consistency with other DOE H_2 programs

Prospective LCA modeling for water-splitting technologies (2: LTE, HTE)

Extensive experience in energy analysis for water-splitting technologies

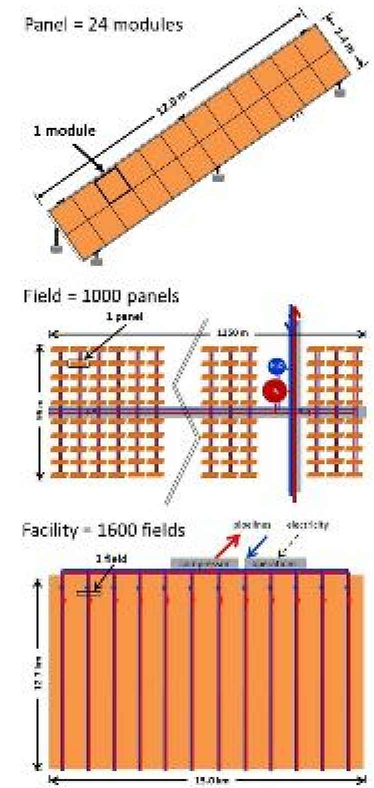
- Estimates of material and energy flows across entire plant life-cycle including total cost of ownership and externalities
- Ability to add costs or other metrics to model

PEC example:

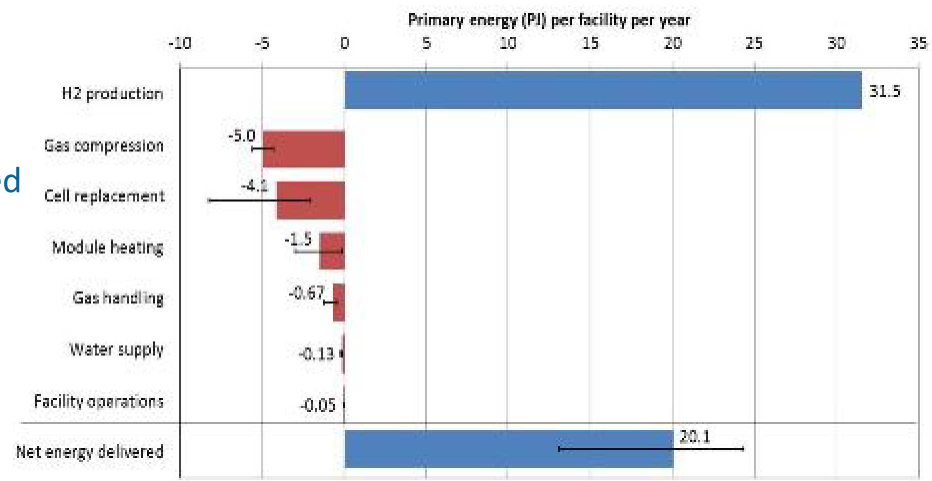


Calculated energy metrics:

- **Net energy**
- **Energy return on energy invested (EROEI)**
- **Energy payback time**



- New materials, components and processes can easily be incorporated
- Perform sensitivity analysis of key parameters
- Monte Carlo simulation capability
- Synergistic with technoeconomic analysis



For more information

Go to www.h2awsm.org

FAQ

Capability node lists and descriptions

Send email to h2awsm@nrel.gov

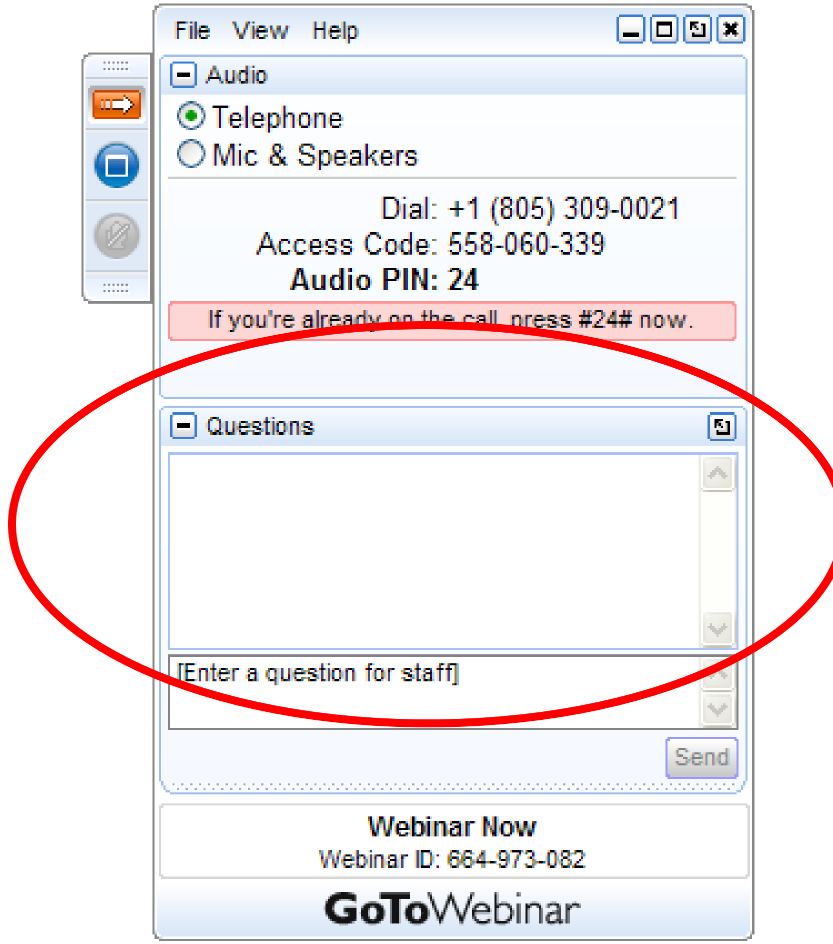
NREL: **Huyen Dinh**	Berkeley Lab: **Adam Weber**	Sandia National Laboratories: **Anthony McDaniel**
INL: **Richard Boardman**	Lawrence Livermore National Laboratory: **Tadashi Ogitsu**	SRNL: **Héctor Colón-Mercado**

Upcoming Webinars on HydroGEN EMN Consortia

Webinar	Links to register for webinar	Date and Time
FCTO's HydroGEN Consortium Webinar Series, Part 1 of 3: Photoelectrochemical (PEC) Water Splitting	https://attendee.gotowebinar.com/register/4254096628056359684	Thursday, November 10th, 2016; 4 – 5 PM EST
FCTO's HydroGEN Consortium Webinar Series, Part 2 of 3: Electrolysis	https://attendee.gotowebinar.com/register/1213908600370749482	Tuesday, November 15th, 2016; 4 – 5 PM EST
FCTO's HydroGEN Consortium Webinar Series, Part 3 of 3: Solar Thermochemical (STCH) Hydrogen Production	https://attendee.gotowebinar.com/register/3983369483529561644	Thursday, November 17th, 2016; 4 – 5 PM EST

Question and Answer

- Please type your questions into the question box



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Thank you

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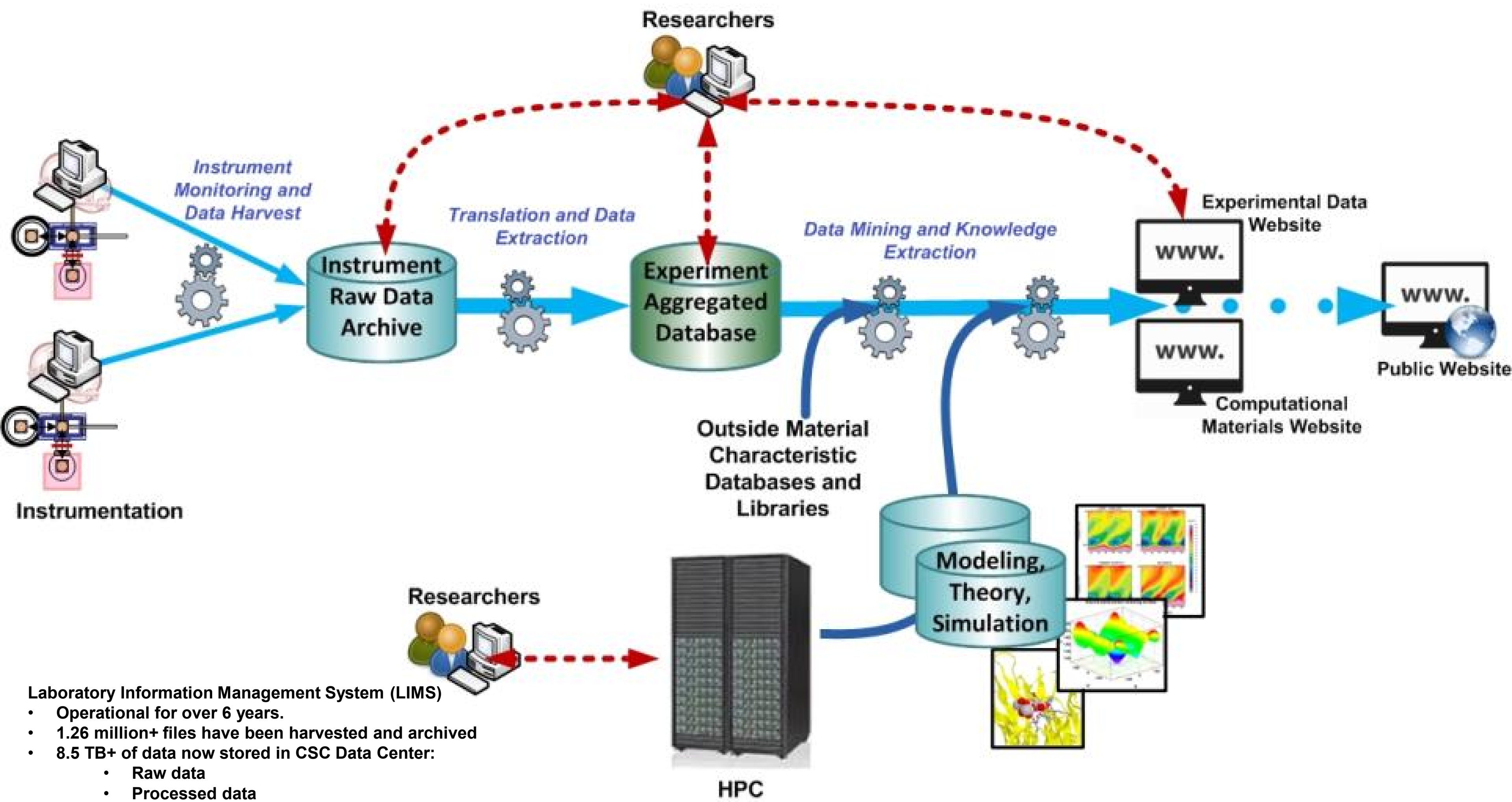
hydrogenandfuelcells.energy.gov

NREL Experimental and Computational Materials Data System (ALL)



Laboratory Information Management System (LIMS)

- Operational for over 6 years.
- 1.26 million+ files have been harvested and archived
- 8.5 TB+ of data now stored in CSC Data Center:
    - Raw data
    - Processed data
    - Associated metadata
    - Simulation and modeling data
- Automated harvesting taking place in 7 labs and over 38 heterogeneous instruments.
- Ability to track samples and experimental projects “cradle to grave”
- Able to automatically process, analyze, or visualize data products in harvesting stream.

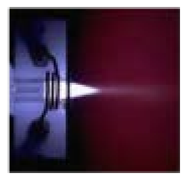
NREL Contamination related capabilities (2: LTE, 3: HTE)

Ion Chromatography [IC]

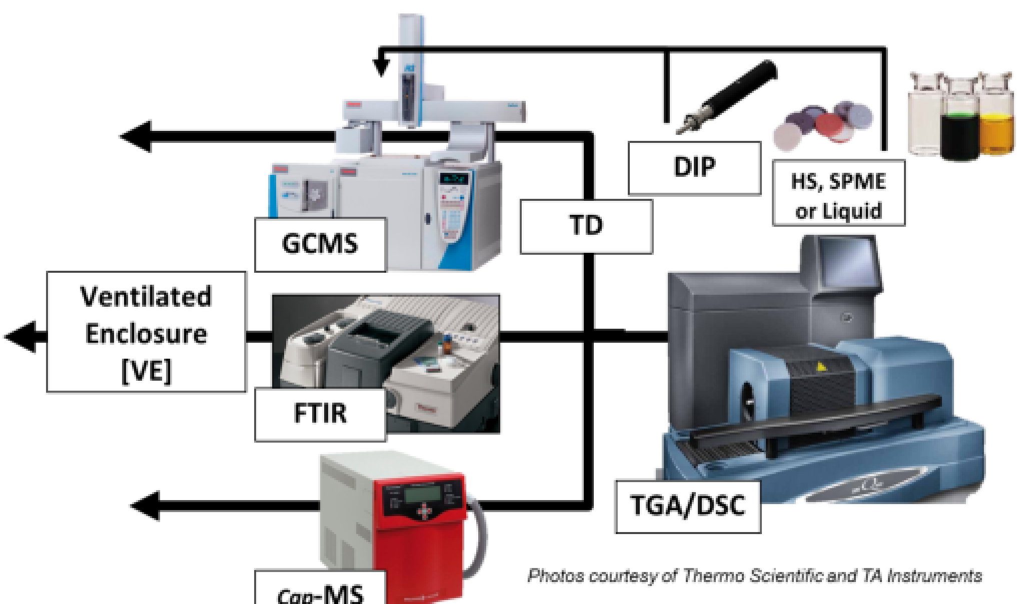
- Dionex ICS 5000
- Separation of ions and polar molecules to determine oxidation state
- Column stationary phase interacts with sample through coulombic interactions
- Ions are measured by Conductivity or UV detectors

Inductively Coupled Plasma [ICP]

- Thermo iCAP Q, with CCT technology
- Trace Elemental Analysis
- Plasma produces excited ions
- Ions are channeled to a mass spectrometer [MS]



Evolved Gas Analysis [EGA]



Photos courtesy of Thermo Scientific and TA Instruments

- Characterize in-situ contaminants effect on fuel cell performance and durability
- Identify and quantify trace leachates and leachate compounds that originate from materials
  - IC, ICP-MS, ICP-OS
  - GCMS with liquids, headspace, and SPME
  - FTIR
  - Total organic carbon (TOC)
- Evolved Gas Analysis using adaptable analytical instrumentation with TG in combination with IR, MS, GCMS

High Flux Solar Furnace (HFSF) (2: HTE)

2

Aerial view of facility

Water splitting reactor

Purpose: NREL's HFSF is ideally suited for small-scale feasibility studies. It is available for on-sun functional component performance testing and materials testing for photo-electrochemical (PEC) cell and STCH solar receiver.

Key Features:

- NREL's HFSF has been in operation since 1990 and consists of a tracking heliostat and 25 hexagonal slightly concave mirrors to concentrate solar radiation.
- The solar furnace can quickly generate over to 1,800°C over a 1-cm^2 area—and up to 3,000°C with specialized secondary optics to generate concentrations greater than 20,000 suns.
- Flux levels and distributions can also be tailored to the needs of a particular research activity.
- The operational characteristics and size of the facility make it ideal for testing over a wide range of technologies with a diverse set of experimental requirements.
- The facility can provide a platform for testing prototype for solar-electric and solar-chemistry applications.

References:

- Martinek, J., Bingham, C., & Weimer, A. W. (2012). Computational modeling and on-sun model validation for a multiple tube solar reactor with specularly reflective cavity walls. Part2: Steam gasification of carbon. Chemical engineering science, 81, 285–297.
- Lichty, P., Liang, X., Muhich, C., Evanko, B., Bingham, C., & Weimer, A. W. (2012). Atomic layer deposited thin film metal oxides for fuel production in a solar cavity reactor. International Journal of Hydrogen Energy, 37(22), 16888-16894.

In-situ and *operando* nanoscale characterization capabilities for photoelectrochemical materials and integrated assemblies

A combination of different AFM techniques able to optimize (photo)electrochemical assemblies

This suite of characterization techniques comprises:

- Peak force AFM (PF-AFM)
- Photoconductive AFM (PC-AFM),
- Kelvin probe force microscopy (KPFM),
- Electrochemical AFM (EC-AFM)
- Photoelectrochemical AFM (PEC-AFM)

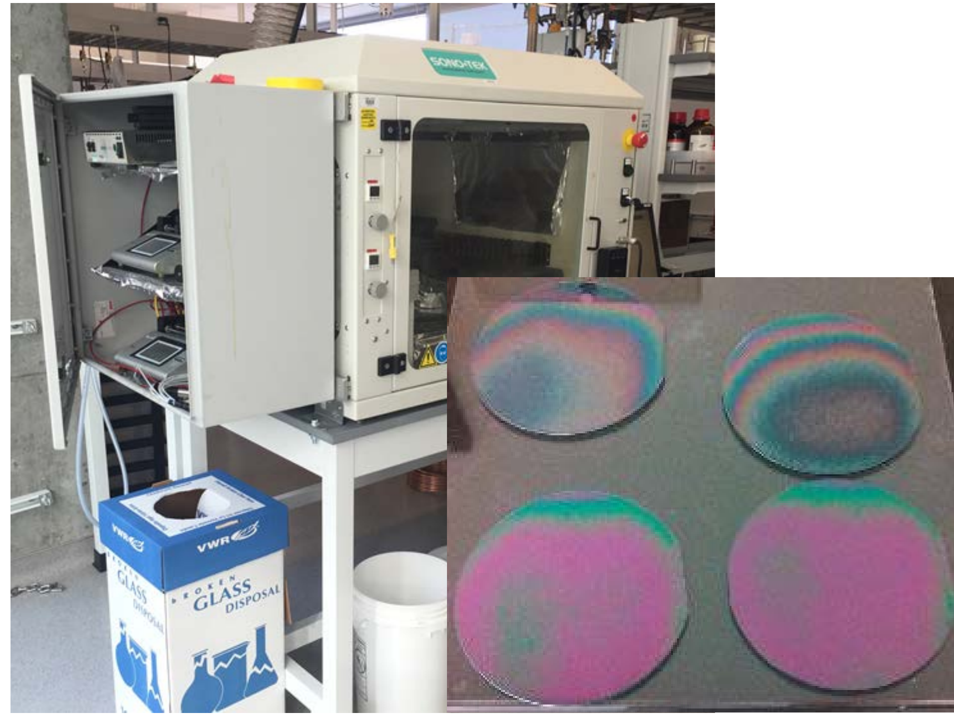
for in-situ and operando characterizations and with associated expertise for data acquisition and analysis

Left: setup for EC-AFM. Right: topography, contact current and electrochemical current of Au squares surrounded by a Si_3N_4 frame. 10 mM $[Ru(NH_3)_6]^{3+}$ solution as electrolyte.

- *In-situ* and *operando* characterization of (photo)electrochemical systems using light illumination including from various lasers.
- These techniques are suitable to directly image local nm-scale PEC activity to understand the electrical mechanisms behind the PEC performance

Spray pyrolysis tool

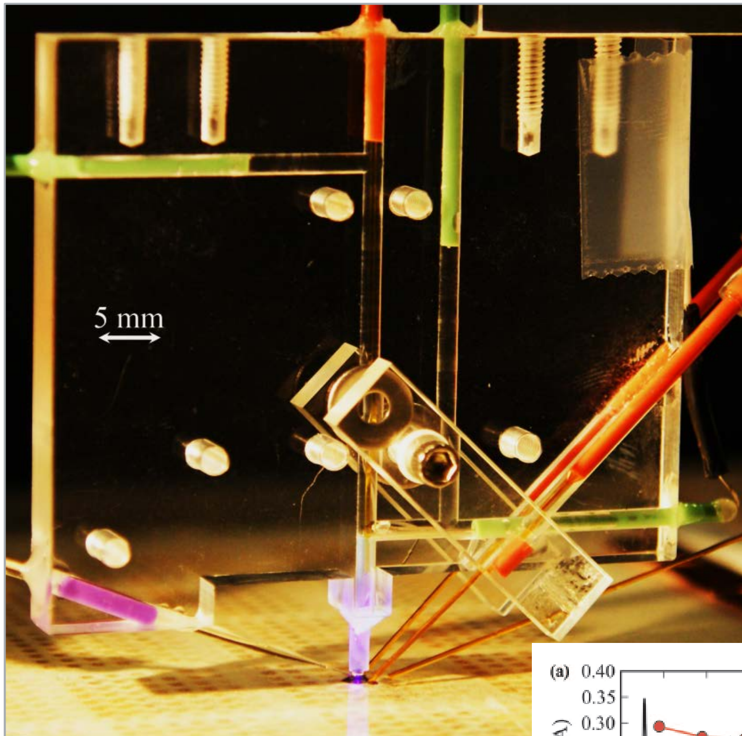
- Fully integrated Sono-Tek spray pyrolysis coating system
  - 2x syringe pumps
    - Ultrasonic and stir bar compatible
  - 2x ultrasonic nozzles
  - Wenesco 9000 W hot plate
    - 12x12 inches
    - Temperature 29 to 600 ^oC
  - Recipes available for transparent conducting oxides and metal oxide films

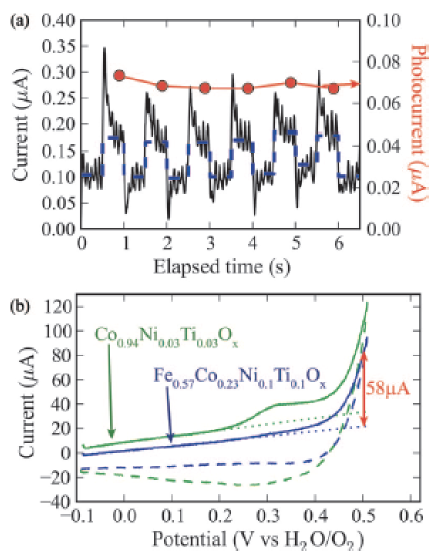


Reference:

K.A. Walczak, Y. Chen, C. Karp, J.W. Beeman, M. Shaner, J. Spurgeon, I.D. Sharp, X. Amashukeli, W. West, J. Jin, N.S. Lewis, and C. Xiang. Modeling, Simulation, and Fabrication of a Fully Integrated, Acid-stable, Scalable Solar-Driven Water- Splitting System, *ChemSusChem* **8**, 544 (2015).

Scanning droplet cell for high throughput electrochemical evaluation



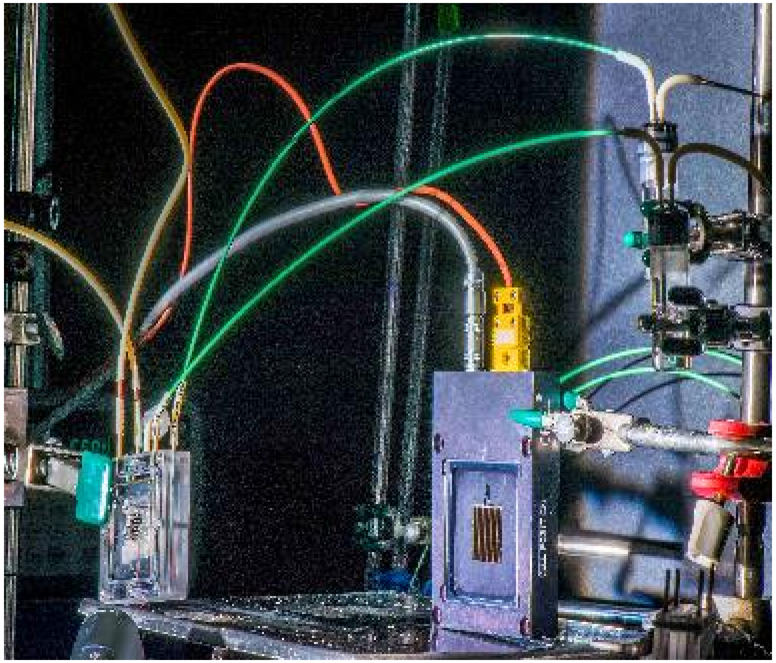


J. M. Gregoire, CX Xiang, X. Liu, M. Marcin, J. Jin, Rev Sci Instrum 2013, 84, 024102

- Programmable raster over large areas
- Provides 3-electrode measurements, compatible with electrolytes across the pH scale
- Fiberoptics allow for PEC evaluation of materials
- Multiple measurements at each location (e.g., cyclic voltammetry, chronoamperometry, chronovoltammetry)
- Droplet constantly refreshed, eliminating cross contamination
- Applicable to a wide variety of high throughput synthesis methodologies
- Capability currently on loan, duplicate to be constructed

Water-splitting device testing

- Electro- and photoelectro- chemical, testing and characterization stations
  - 30 x 30 cm Oriel Sol3A solar simulator (model: SP94123A-5354, vendor: Newport) with dose exposure control, and calibrated Si reference cell
  - 2x channel gas chromatography
    - 50 ppm sensitivity for hydrogen and oxygen
  - Inverted-burette with digital manometer for production rate
  - Biologic potentiostats with impedance, computer system, and video camera
  - High current power supplies and various testing hardware
  - Multiple Scribner and Fuel Cell Technologies test stations outfitted for electrolysis and Maccor Battery Cycler (up to 120A)
  - Various cell assemblies and architectures

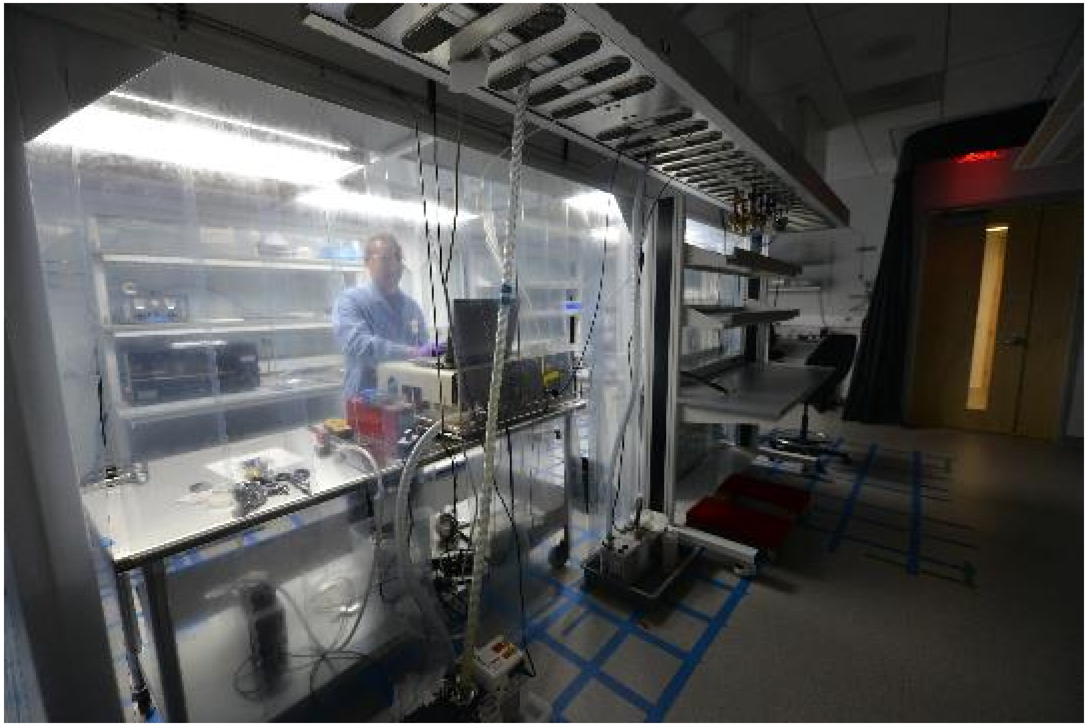


Cleanrooms with surface preparation

2 cleanrooms with facilities for surface cleaning and coating, sizes up to 150 mm

Room 1, softwall cleanroom in dedicated lab:

- GEMSTAR-6 Thermal Atomic Layer Deposition tool (model: GEMSTAR-6, vendor: Arradiance) for depositing highly conformal thin films with precise control of composition and thickness at relatively low temperatures (40 to 300^{o}C)
- Plasma cleaner (model: PDC-32G, vendor: Harrick Plasma) and UV-ozone cleaner for removal of surface impurities
- Vacuum desiccator
- CO_2 sno-gun for particle removal
- Anti-static work surfaces
- Ellipsometer for film thickness measurements
- Custom large area optical-inspection tool for finding and mapping surface defects at the micron scale over large areas

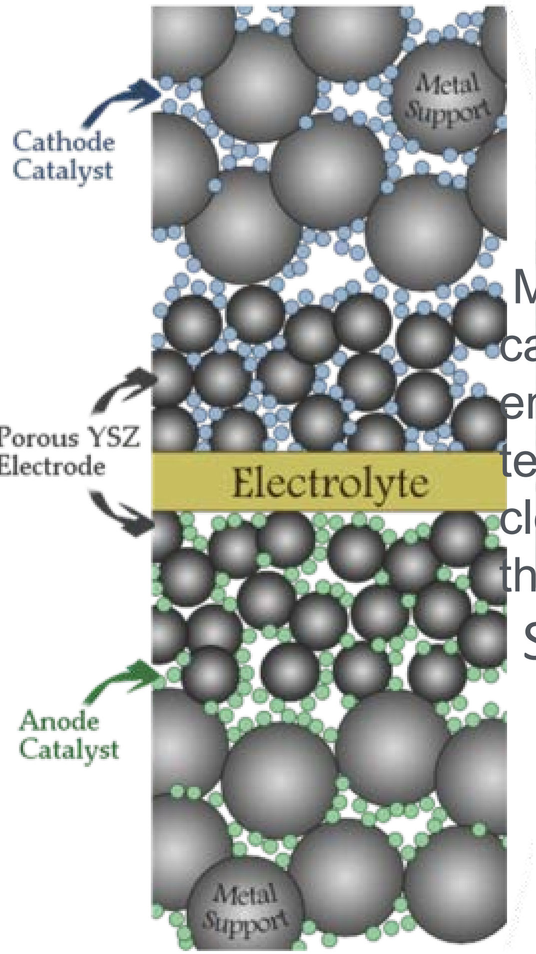


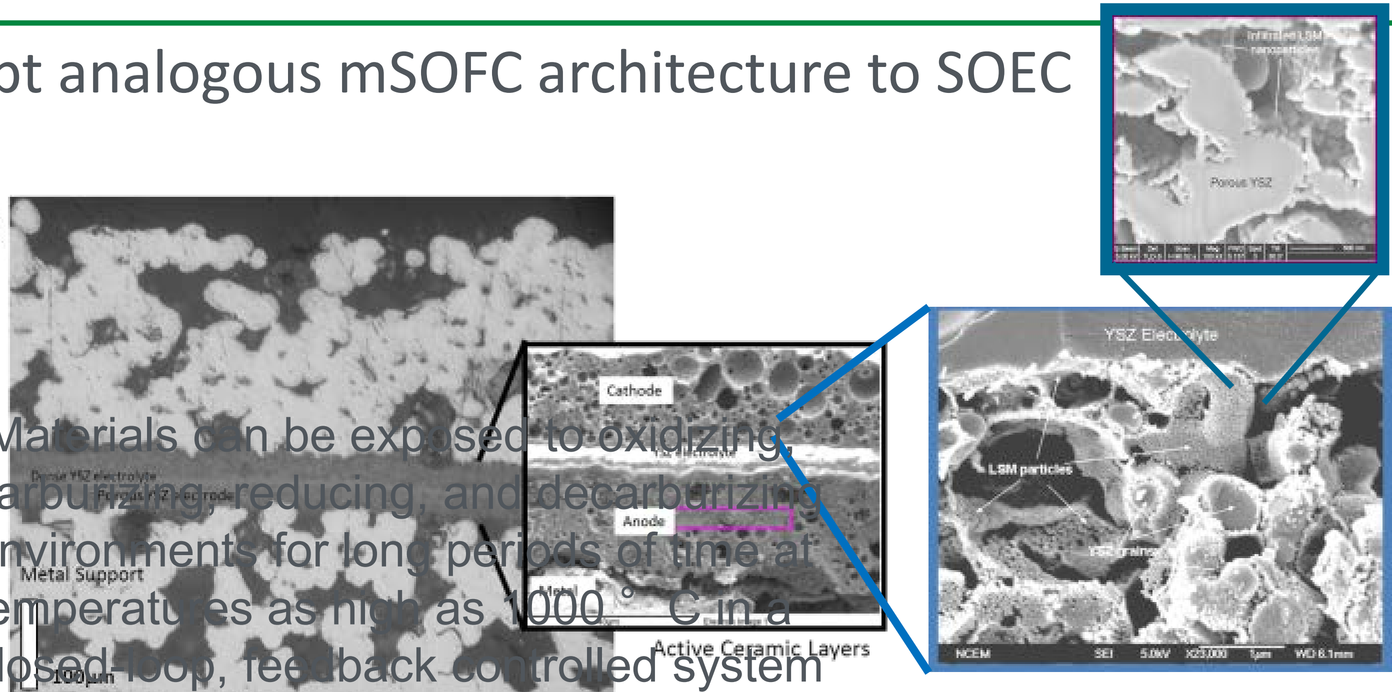
Room 2, dedicated wet process and assembly cleanroom:

- Wet benches for solvent and acid cleans including HF
- Laminar flow hood for substrate and component assembly and packaging

Metal-Supported Solid Oxide Electrolysis Cell (mSOEC)

Opportunity to adapt analogous mSOFC architecture to SOEC





Nanocatalysts covering porous YSZ electrolyte

Materials can be exposed to oxidizing, carburizing, reducing, and decarburizing environments for long periods of time at temperatures as high as 1000 °C in a closed-loop, feedback controlled system that pre-mixes the gas environment.

Synthesis, testing, and analysis expertise and equipment

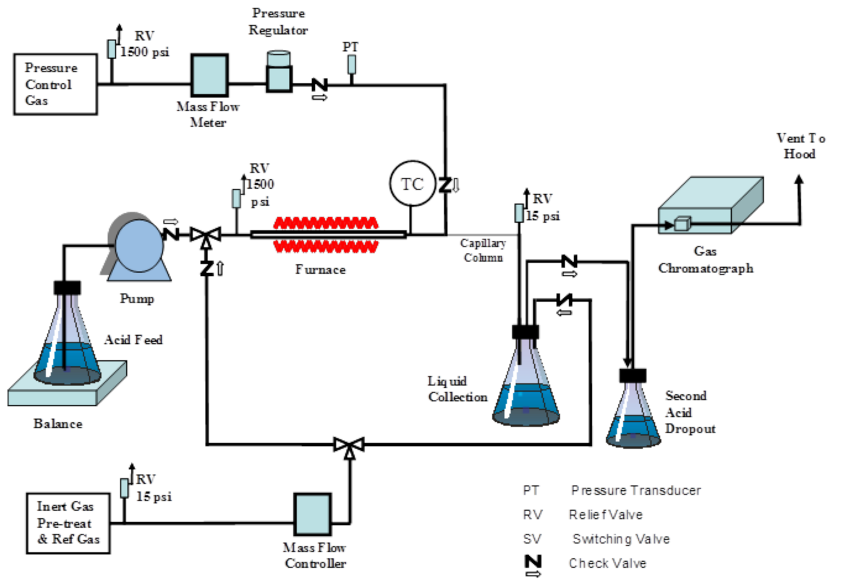
Rugged, low-cost stainless steel mechanical support

- Robust thermal shock tolerance

Infiltrated nano-catalysts

- Power density >1 W/cm^2 at 700°C
- Rapid screening and implementation of new catalysts

Catalysts for Harsh Environments (2: HT)



INL Pressurized Catalyst Test System

Purpose: This node develops and evaluates catalysts for thermochemical water splitting cycles, such as the Sulfur-Iodine and Hybrid Sulfur cycles.

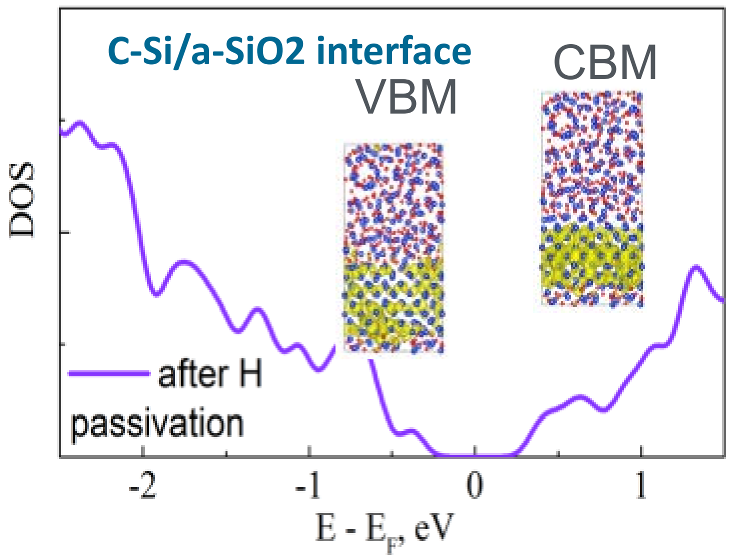
INL's Key Features:

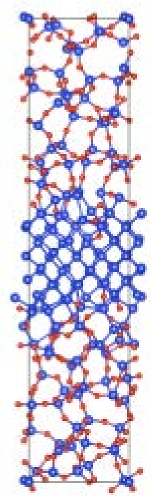
- Laboratory set up and techniques for catalyst development and evaluation under harsh conditions that are common to high temperature water-splitting chemical loops; e.g., sulfuric acid dissociation, and HI solution splitting
- Multiple catalyst evaluation systems for harsh environments
- Capabilities of up to 50 grams catalyst, pressure to 30 bar, 1300 K, WHSV 50 grams acid/gram catalyst/hour with testing for thousands of hours of operation
- Continuous-flow and catalysis performance monitoring for hundreds to thousands of hours
- Over 100 unique catalysts evaluated for sulfuric acid splitting and hydroiodic acid splitting reactions
- Collaborations with catalyst manufacturer Johnson Matthey, National Laboratories (SRNL, SNL, PNNL) and scale-up partner GA

High Temperature Materials Degradation and Corrosion Characterization and Mitigation for H_2 Production (3: HT, HTE)

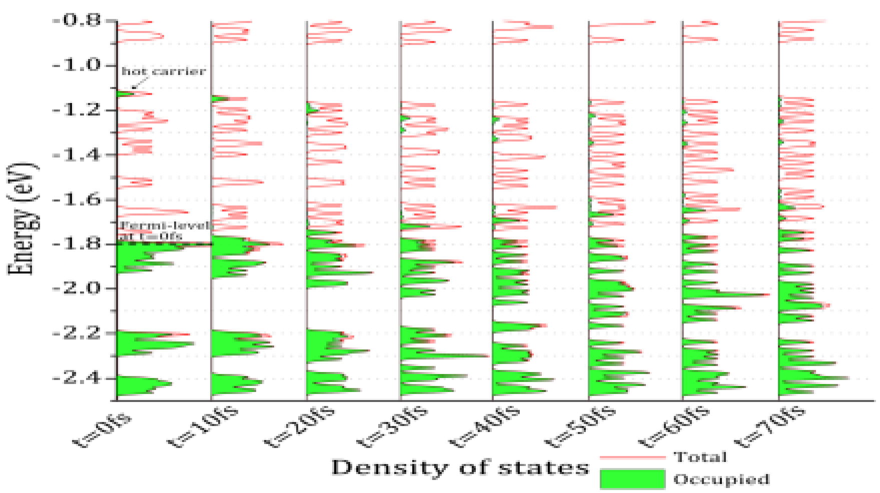
- Electrochemical testing cells, immersion tests, and thermosiphon flow testing capabilities in walk-in hood
- Thermosiphons furnaces have three heating zones for temperature/flow velocity control
- Gas manifolds to ensure negligible or controlled introduction of impurities to cells
- Gloveboxes for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

Ab initio simulation of amorphous protection layer and rt-TDDFT simulation of carrier dynamics





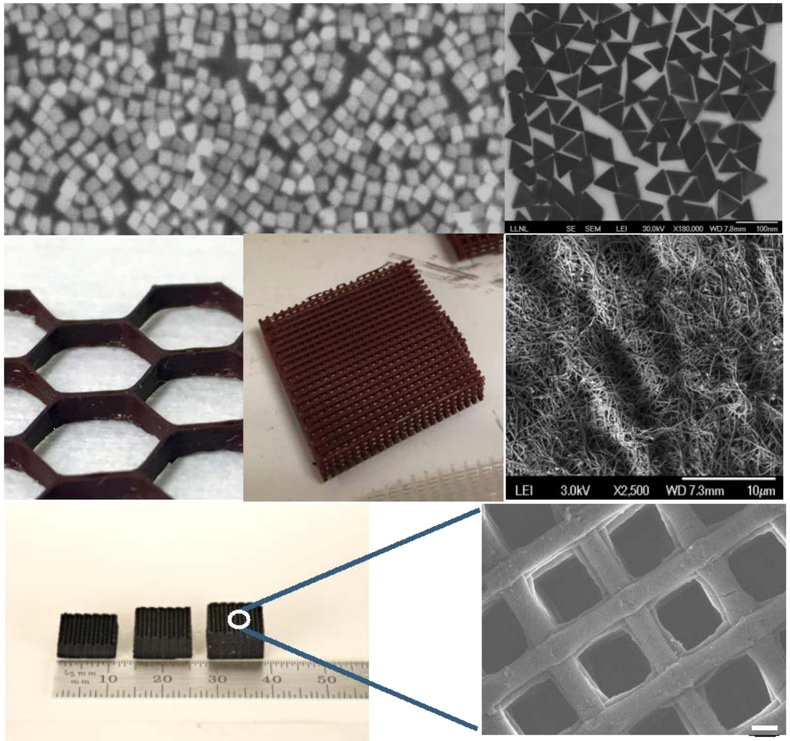
Hot-carrier cooling in Al nanocluster



- Ab initio simulation of amorphous oxides electronic structures and defect states
- Using Marcus theory to calculate electron transport between trap states
- Linear scaling 3 dimensional fragment (LS3DF) method for DFT calculation of large (>10,000 atom) systems
- New algorithms for rt-TDDFT allowing calculation of carrier transport and other excited state dynamics for systems with hundreds of atoms for hundreds of fs

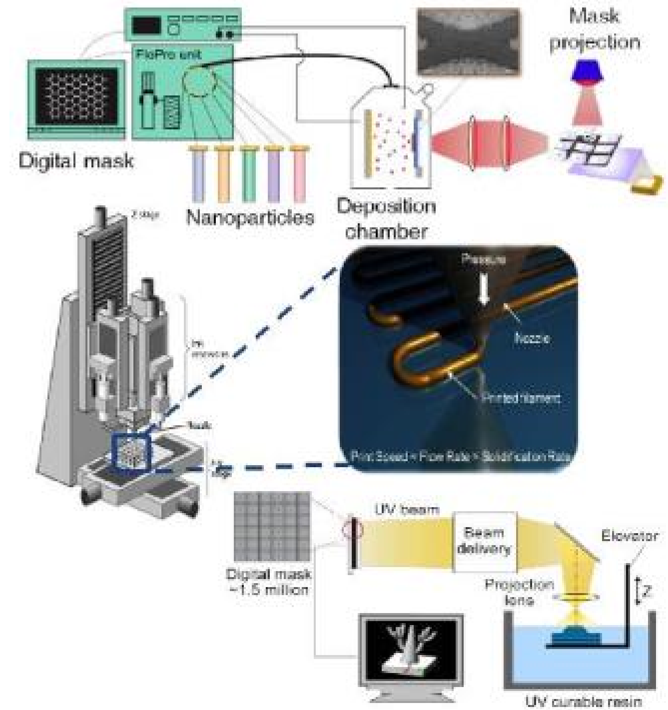
DFT applied for PEC and EC (ORR) but can be adapted for other technologies

Fabrication of Custom Electrodes at Multiple Length Scales using Additive Manufacturing (All Cat 2)



Custom Materials Synthesis

Scale-Up

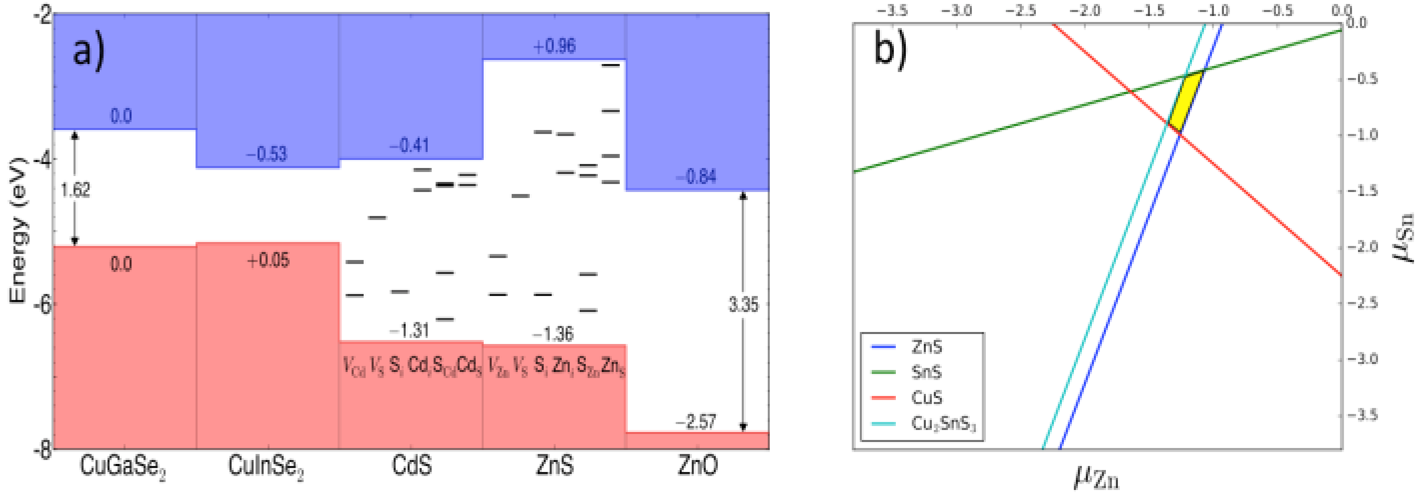


Additive Manufacturing

Combining abilities to ***synthesize*** and ***scale-up*** custom materials (i.e. conductive high surface area electrodes/catalysts) to formulate unique feedstock materials for ***additive manufacturing*** processes, including direct-ink writing, electrophoretic deposition and projection micro-sterolithography, opens up design space to create optimized catalysts and electrodes for water splitting.

Computational Materials Diagnostics and Optimization of Photoelectrochemical Devices (2: LTE)

Varley and Lordi, J. App. Phys. 116, 063505 (2014)



Provide: (DFT/Hybrid functional/GW level)

- **Band alignment**
- **Character (malignant/benign) and position of gap levels**
- **Thermodynamics stability of alloys for a given condition (μ, T)**
- **Defect thermodynamics for a given condition (μ, T)**

Optimal choice of absorber/buffer pair including synthesis/process condition that minimizes detrimental effect