Fuel Cell Technologies Office Webinar

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

HydroGEN – AWSM:

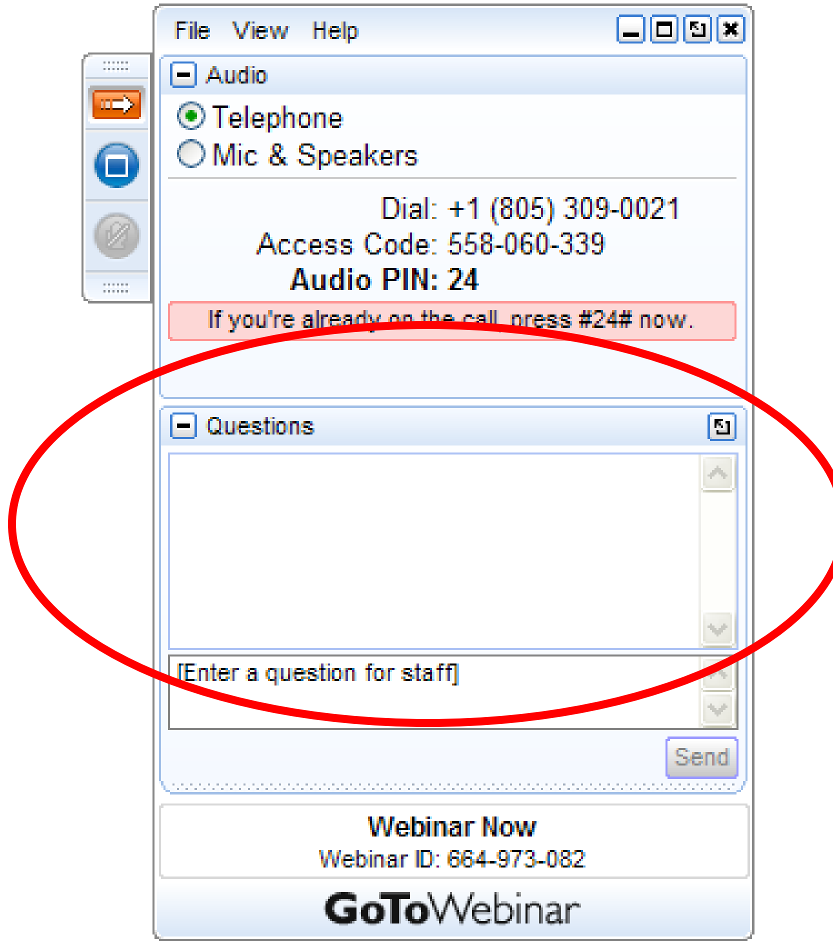
Solar Thermochemical (STCH)

November 17, 2016

Anthony McDaniel
Technical Staff
Sandia National Laboratories

Question and Answer

- Please type your questions into the question box



Energy Materials Network
U.S. Department of Energy

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?

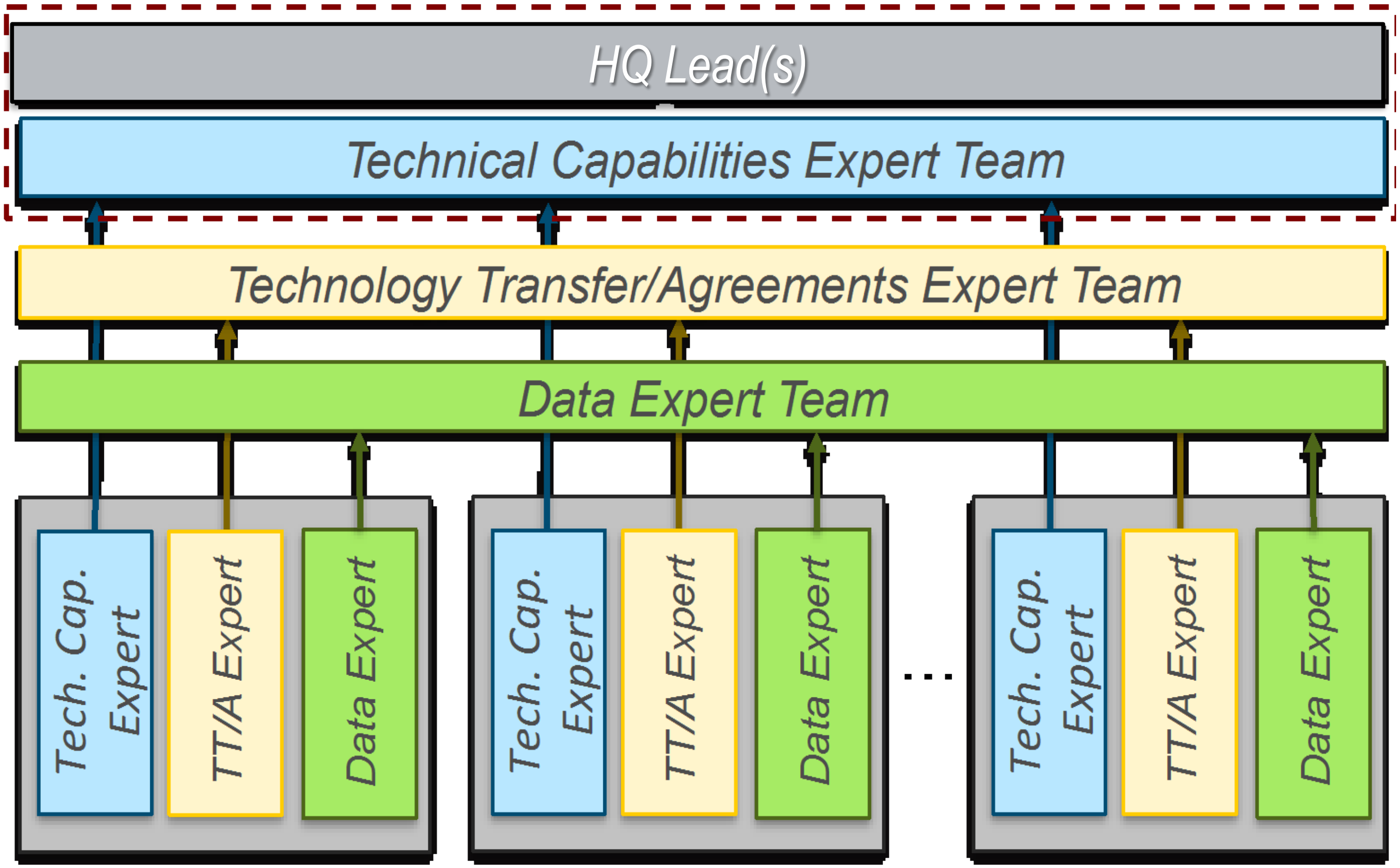
The EMN offers a common yet flexible RD&D consortium model to address key materials challenges in specific high-impact clean energy technologies aimed at accelerating the tech-to-market process

Consortium Requirements

- **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.*

Ensuring Transparency

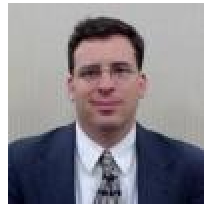
Consortium Steering Teams



HydroGEN Steering Committee

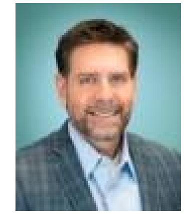
NREL
NATIONAL RENEWABLE ENERGY LABORATORY

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

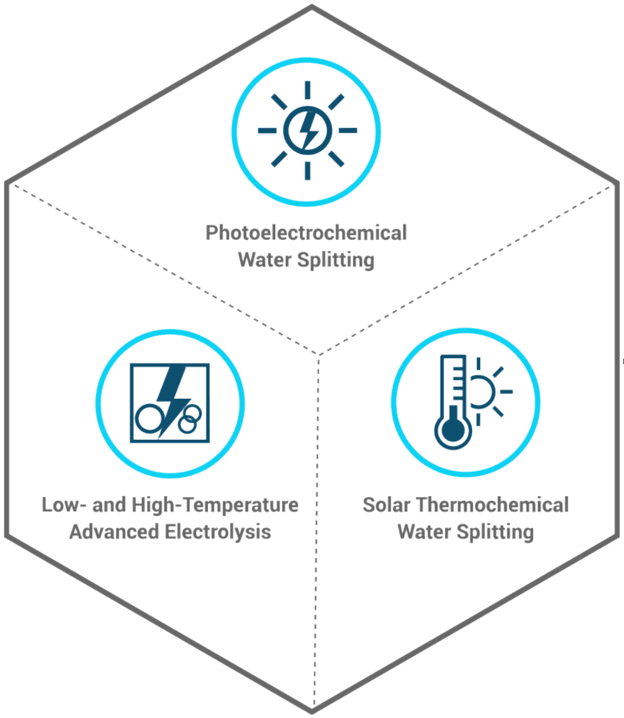
Eric Miller, DOE-EERE-FCTO

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** *:*

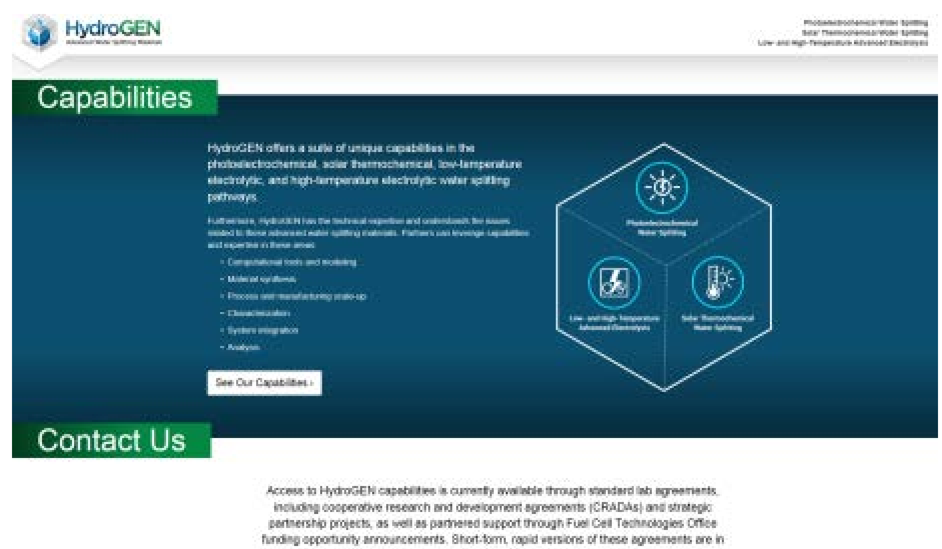
Advance Electrolysis	Photoelectrochemical	Solar Thermochemical
Low & High Temperature		Hybrid thermochemical

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)



https://www.h2awsm.org/

Technology Abbreviations:

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

Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

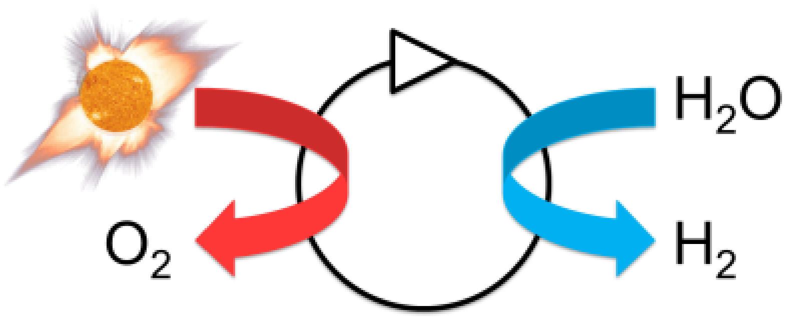
Part 3 of 3: Solar Thermochemical

Anthony McDaniel, Huyen N. Dinh, Héctor Colón-Mercado
November 17, 2016
FCTO Webinar

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

Approaches to STCH hydrogen

Thermochemistry



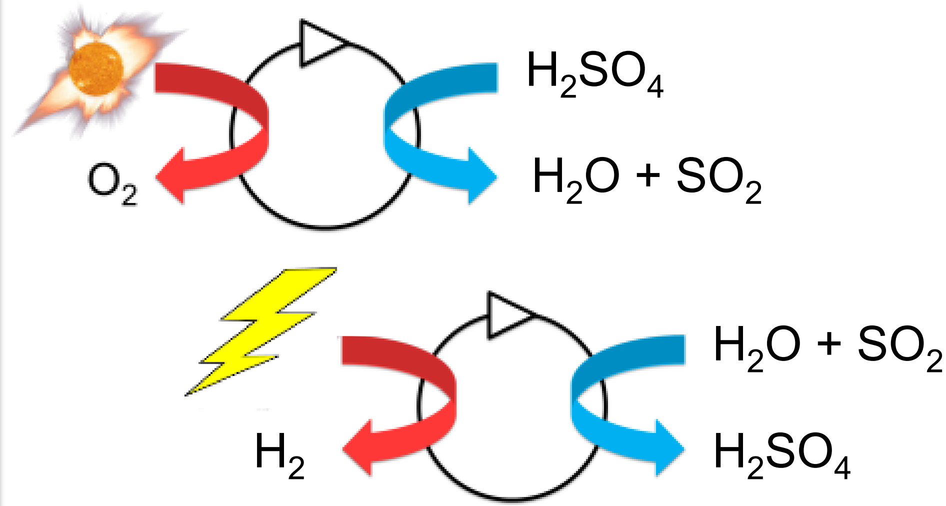
$$MO_x \rightarrow MO_{x-\delta} + \frac{\delta}{2} O_2 \qquad \text{(1) Reduction}$$

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

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

- Metal cation is redox active element in two-step cycle

TC + Electrochemistry



$H_2SO_4 \leftrightarrow H_2O + SO_2 + ½ O_2$
(thermochemical; 800-900 °C)
$SO_2 + 2 H_2O \rightarrow H_2SO_4 + H_2$
(electrochemical; 80-120 °C)
Net Reaction: $H_2O \rightarrow H_2 + ½ O_2$

- Sulfur is redox active element in two-step cycle

Conditions and system metrics for MO_x cycle

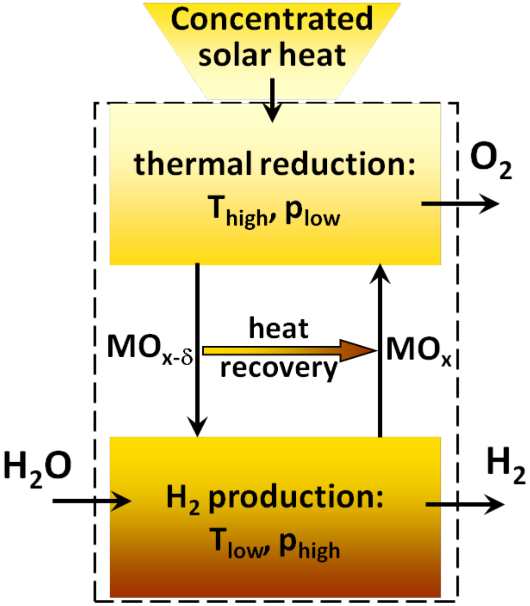
$$MO_x \rightarrow MO_{x-\delta} + \frac{\delta}{2} O_2$$ (1) Reduction

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

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

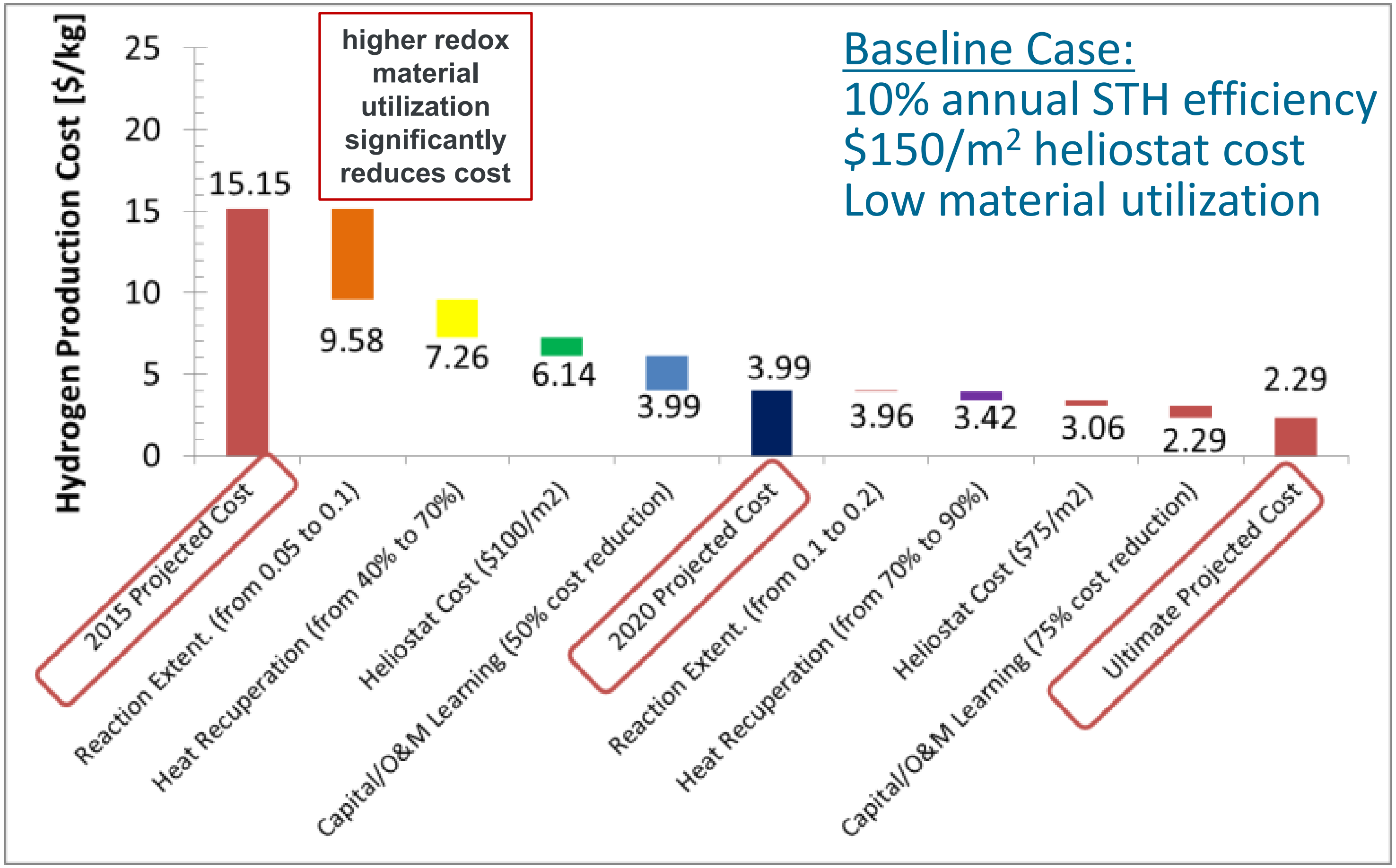
MW scale concentrating solar power facilities provide heat

Reduction Temperature (T_{high})	<2000ºC
"O" activity in reduction (p_{low})	$\mu_{gas} < \mu_{solid}$
Oxidation Temperature (T_{low})	debated
"O" activity in oxidation (p_{high})	$\mu_{gas} > \mu_{solid}$
H_2 production rate	50-100mt/day
Solar-to-H_2 conversion efficiency	>25%
H_2 production cost (US DOE)	\$2-4/kg H_2 dispensed



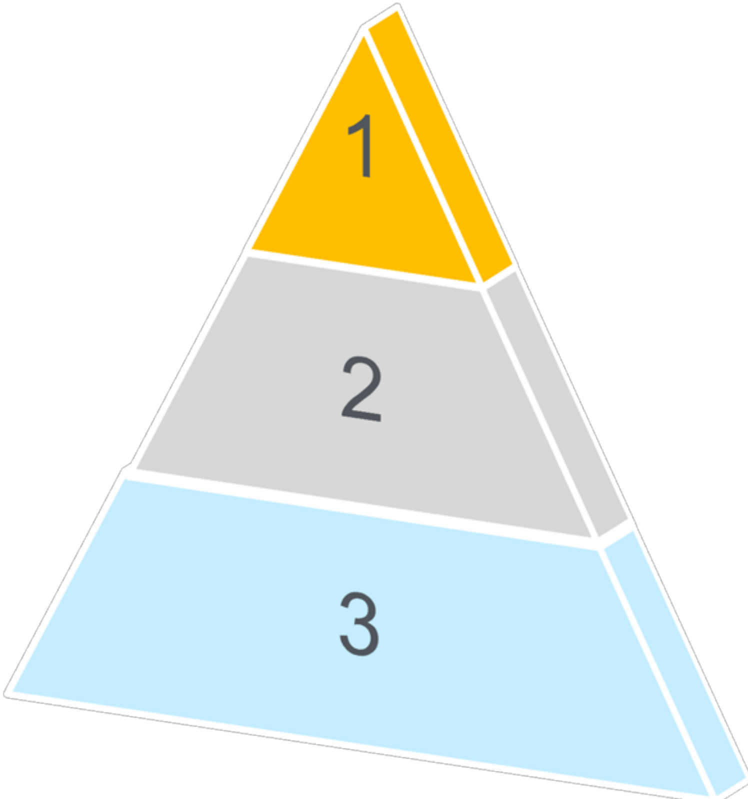
Two-step metal oxide cycle

Waterfall chart: one pathway to meet STCH H_2 cost target for MO_x cycle



Waterfall chart projecting cost reductions in STCH hydrogen production by making serial iterations with a Sandia case study for a 100mt H_2/day centralized plant showing anticipated progress towards technical targets.

Node readiness category chart



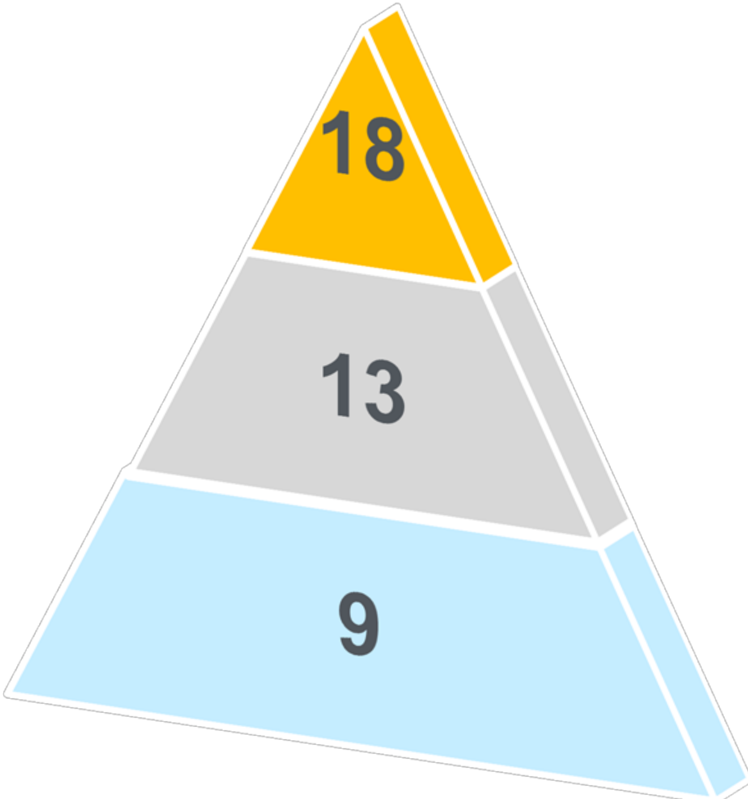
Category 1
Node is fully developed and has been used for STCH research projects

Category 2
Node requires some development for STCH

Category 3
Node requires significant development for STCH

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

40 STCH nodes



Classification:

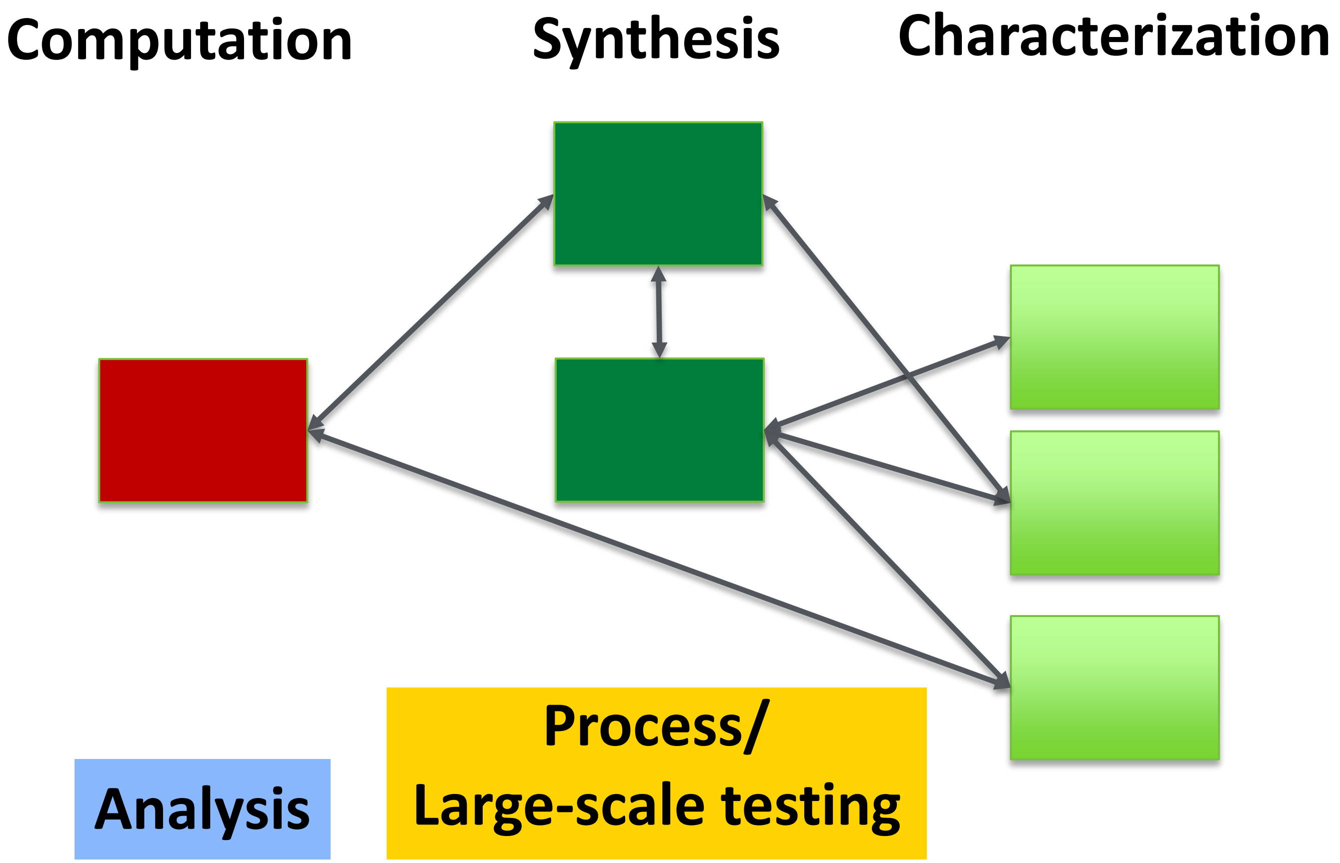
Analysis: 1	Characterization: 5
Computation: 6	Synthesis/Process: 6

Analysis: 1	Characterization: 3
Computation: 5	Synthesis/Process: 4

Analysis: 1	Characterization: 4
Computation: 4	Synthesis/Process: 0

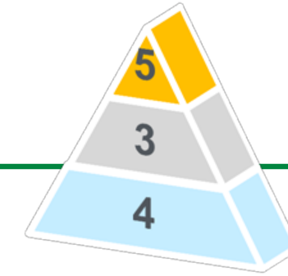
- Nodes comprise tool, technique, and expertise including uniqueness
- Category refers to availability, readiness and relevance to STCH and not necessarily the expense and time commitment
- Note that many nodes span classification areas (analysis, synthesis, computation, characterization, etc.)

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

Characterization Capabilities



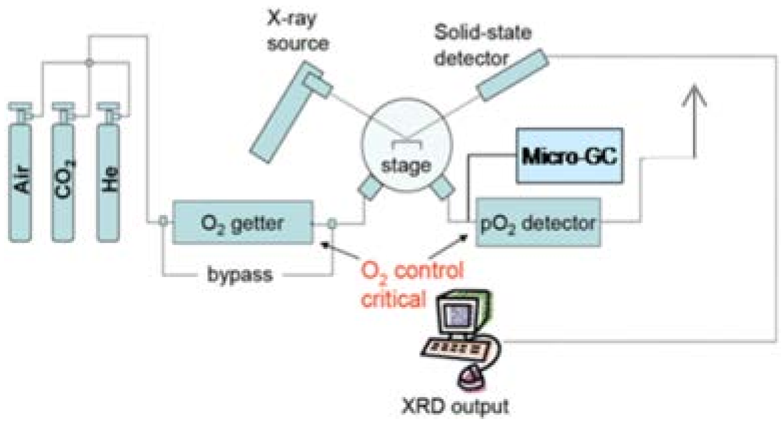
1. High temperature in situ X-ray diffraction, SIMS, & thermal analysis
2. Virtually-accessible stagnation flow reactor
3. Advanced electron microscopy (FIB-SEM-TEM)
4. High temperature catalyst and acid electrolyzer characterization
5. In situ & operando X-ray spectroscopy

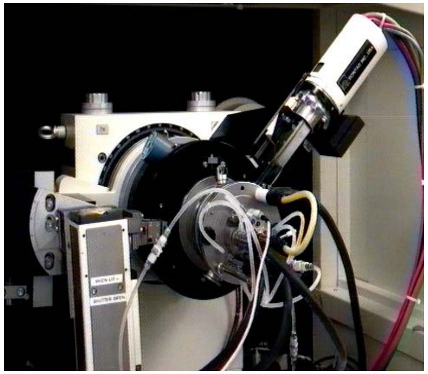
1. Temporal analysis of products (TAPS) reactor system
2. Surface analysis cluster tool
3. Secondary Ion Mass Spectrometry (SIMS)

1. Contamination related capabilities
2. Ex situ spatial characterization for component integration
3. Corrosion analysis of materials
4. Lab-based ambient pressure XPS

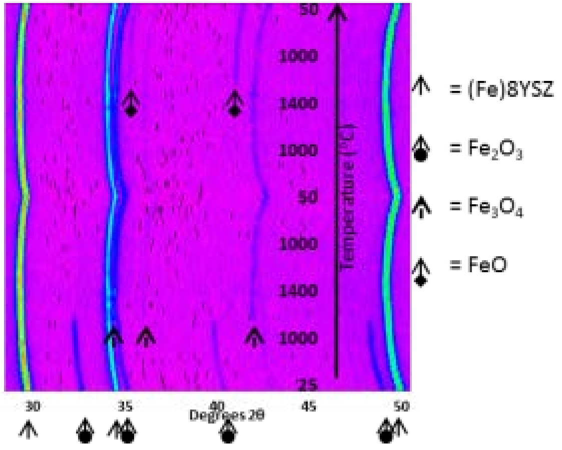
Note that many capabilities span different classification areas and techniques

High temperature in situ X-ray diffraction, ToF-SIMS, & thermal gravimetric analysis

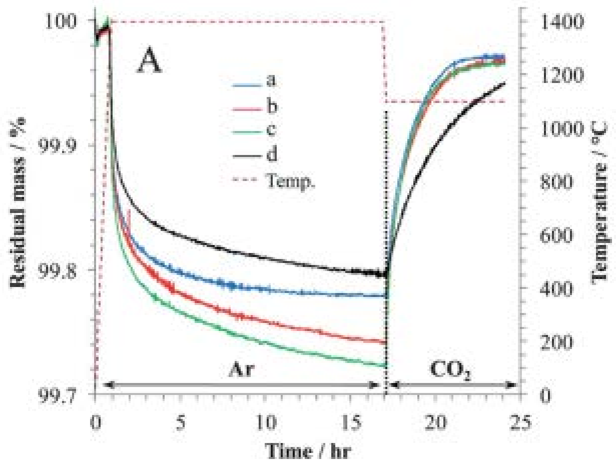


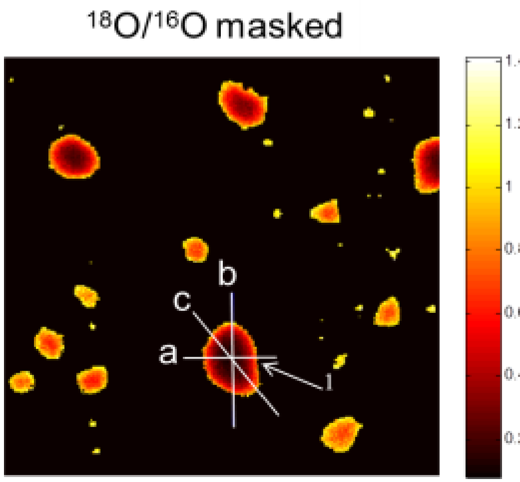


Expertise combining in situ, high temperature X-ray diffraction, thermal analysis, and isotopic labeling of oxygen exchange to uncover mechanistic details of gas splitting



derive structural and mechanistic information using advanced diagnostics (i.e., HTXRD, ToF-SIMS)

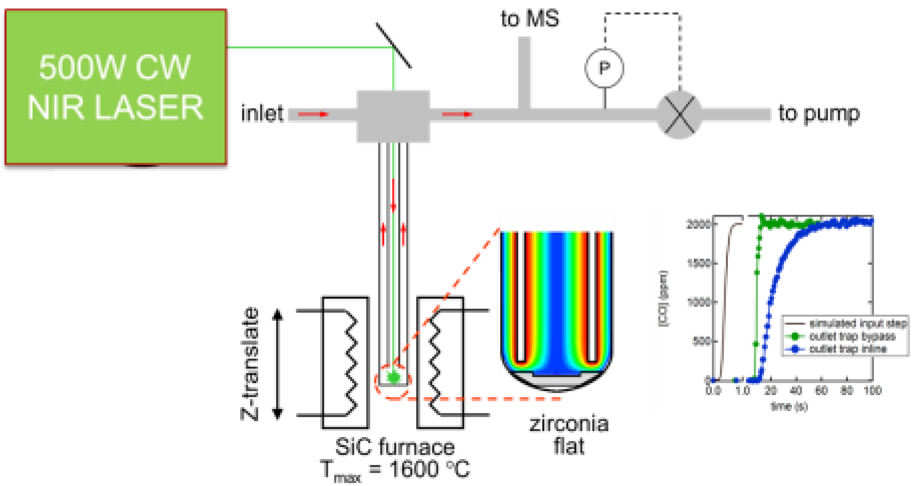


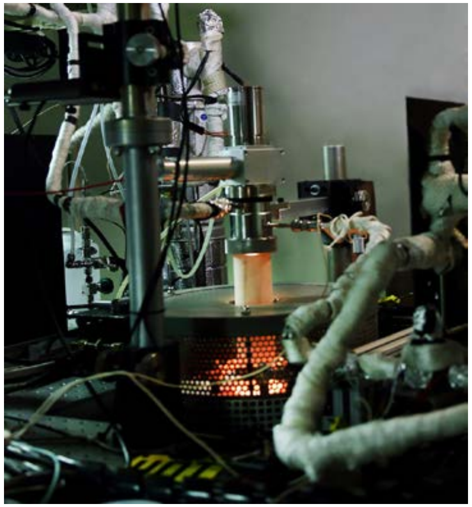


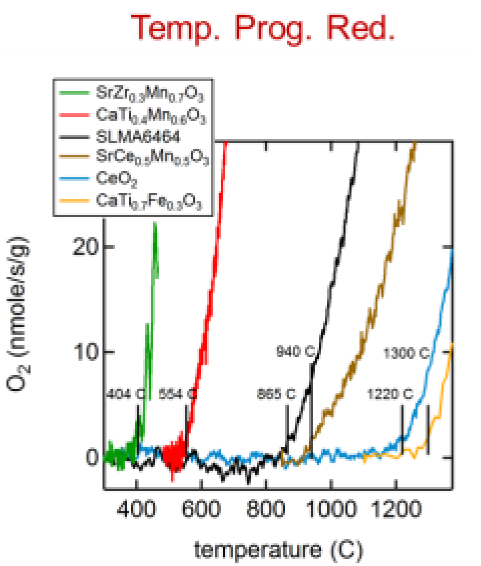
ToF-SIMS of O isotopes reveals <u>muted redox chemistry at phase-segregation boundaries</u>

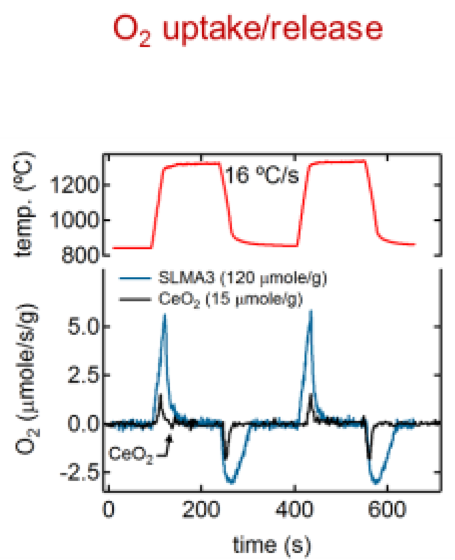
Laser heated stagnation flow reactor for characterizing redox materials under extreme conditions

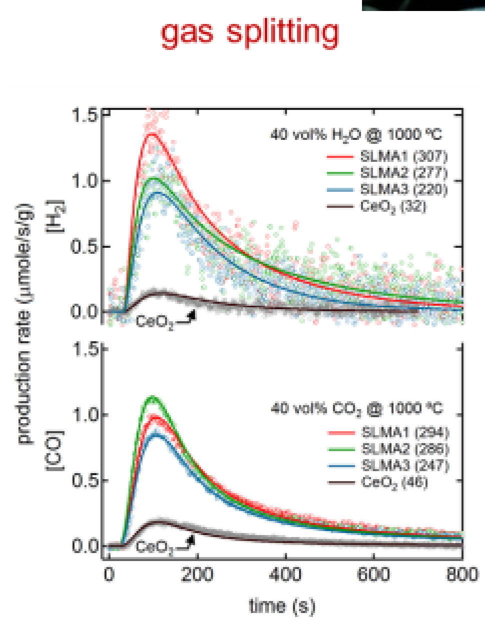
Measure reduction and oxidation rates under high radiative flux and rapid heating rates to <u>resolve detailed kinetics under extreme conditions</u>











Laser-SFR reactor platform is <u>automated and virtually accessible</u> through remote windows desktop

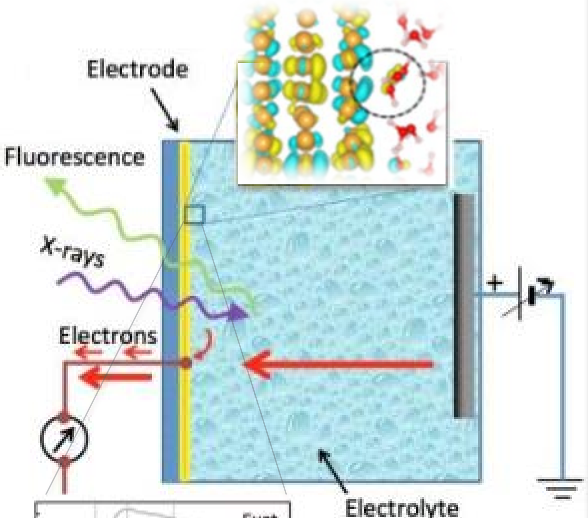
High temperature catalyst and acid electrolyzer component characterization

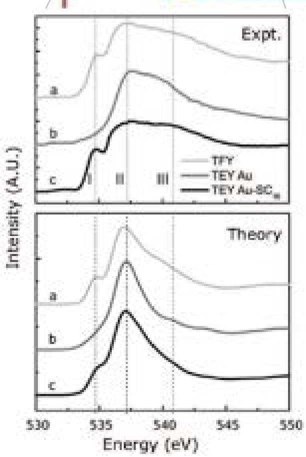
Allows testing components (catalyst and membrane) and membrane electrode assembly collective properties for non-conventional electrolysis

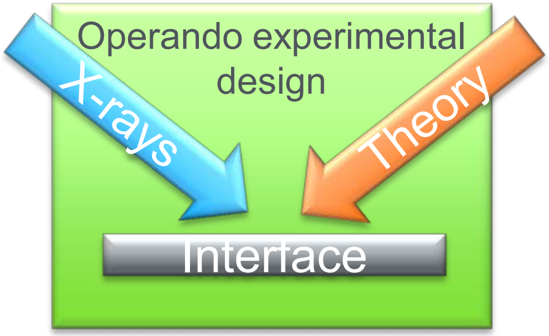
- <u>Catalyst test station</u>-Ex-situ kinetic study of supported catalysts and physical vapor deposited materials on substrates
- <u>Membrane test station</u>-Electrochemical measurement of reactant crossover
- <u>Pressurized Button Cell Test Facility</u>-designed to withstand operation with highly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

X-ray approaches for understanding (photo)electrochemistry at interfaces

Operando XAS



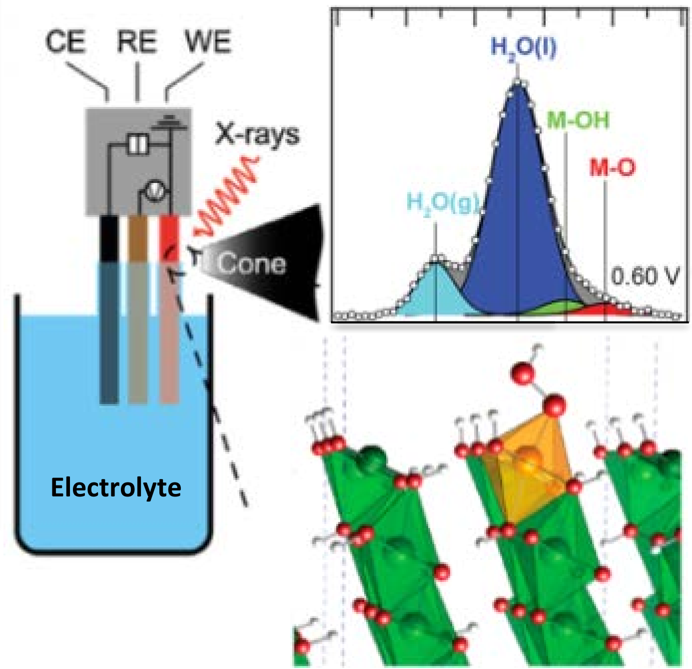




Expertise combining operando instrumentation, X-ray spectroscopy, and theory to uncover molecular-scale chemical details at operating electrode interfaces

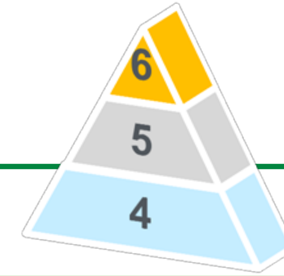
X-ray absorption spectroscopy, coupled to theory, reveals <u>electronic and atomic structure of chemical species</u> at electrode interface

Operando ambient pressure XPS



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

Computation Capabilities



1. Multiscale modeling
2. Albany: Open-source multiphysics platform
3. Computational and experimental tools for enhanced STCH
4. LAMMPS: open-source MD code
5. Uncertainty quantification in computational models
6. Experimental and computational materials data infrastructure

1. Moab: particle-based mesh-free code for modeling transport & phase transition
2. Multiscale modeling of WS devices
3. Mesoscale kinetic modeling of WS and corrosion
4. Time-dependent DFT & ab initio calculations for WS

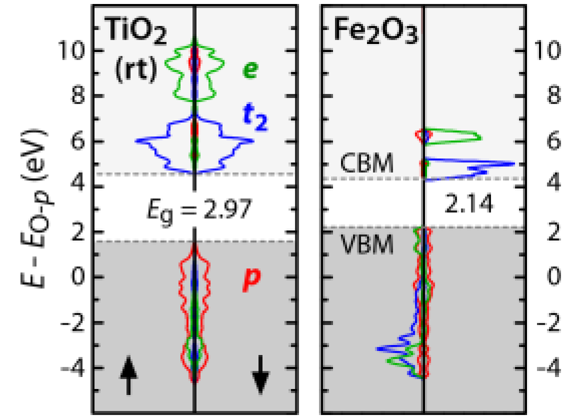
1. Computational materials diagnostics and optimization of PEC devices
2. First principles materials theory for reaction pathways
3. Socorro: code for highly scalable DFT of extended systems
4. Engineering BOP for High temperature systems
5. STCH efficiency prediction platform

Note that many capabilities span different classification areas

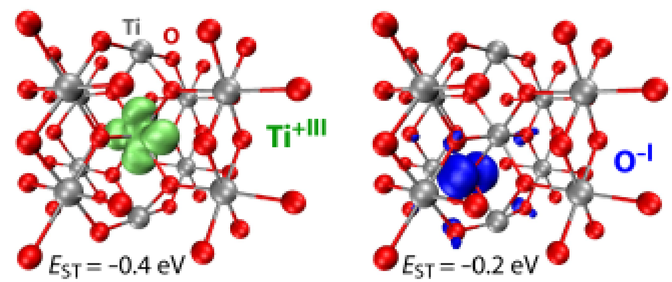
Ab initio, multiphysics, other

First principles materials theory for advanced water splitting pathways

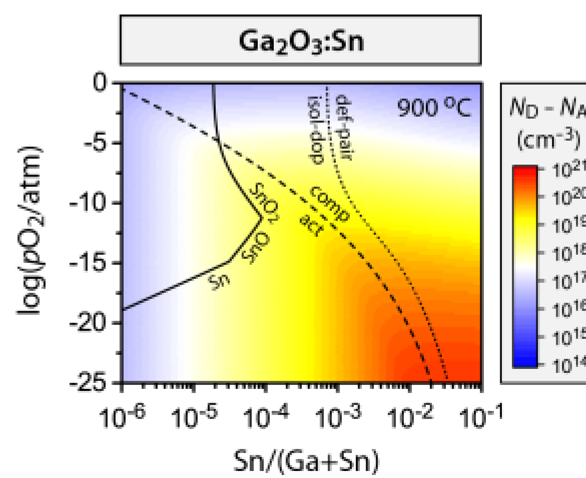
- Electronic structure prediction
  - Accurate band gap prediction for semiconductors, including transition metal compounds
  - Band-structure, effective masses, density of states, ionization potential, band offsets, optical properties



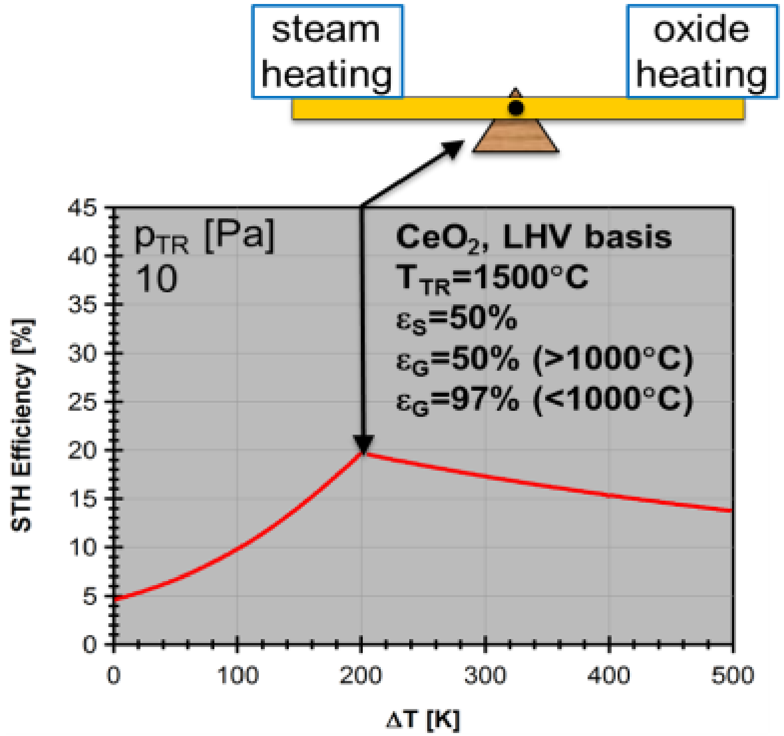
- Defects and alloys
  - Defect equilibria from first-principles, including effects due to defect-pair association
  - Small-polaron transport vs band-like transport
  - Alloys: Mixing enthalpy and phase diagrams
  - Ionic diffusion pathways, energy barriers



- Materials Design and Discovery
  - Structure prediction for new compounds
  - Thermodynamic stability range



STCH efficiency prediction platform



p_{TR}= O_2 reduction pressure
ε_S= solid heat recovery effectiveness
ε_G= gas heat recovery effectiveness

$$\eta = \left(\frac{P_{TH}}{P_S}\right)\left(\frac{LHV_{H_2}}{Q}\right) = \frac{\dot{n}_{H_2} LHV_{H_2}}{P_S} \rightarrow \dot{n}_{H_2} = \frac{P_{TH}}{Q}$$

$$P_{TH} = r_{12} * r_d * t_W * A * P_S - P_{rad}$$

$$Q = Q_{TR} + Q_{SH} + Q_{AUX}$$

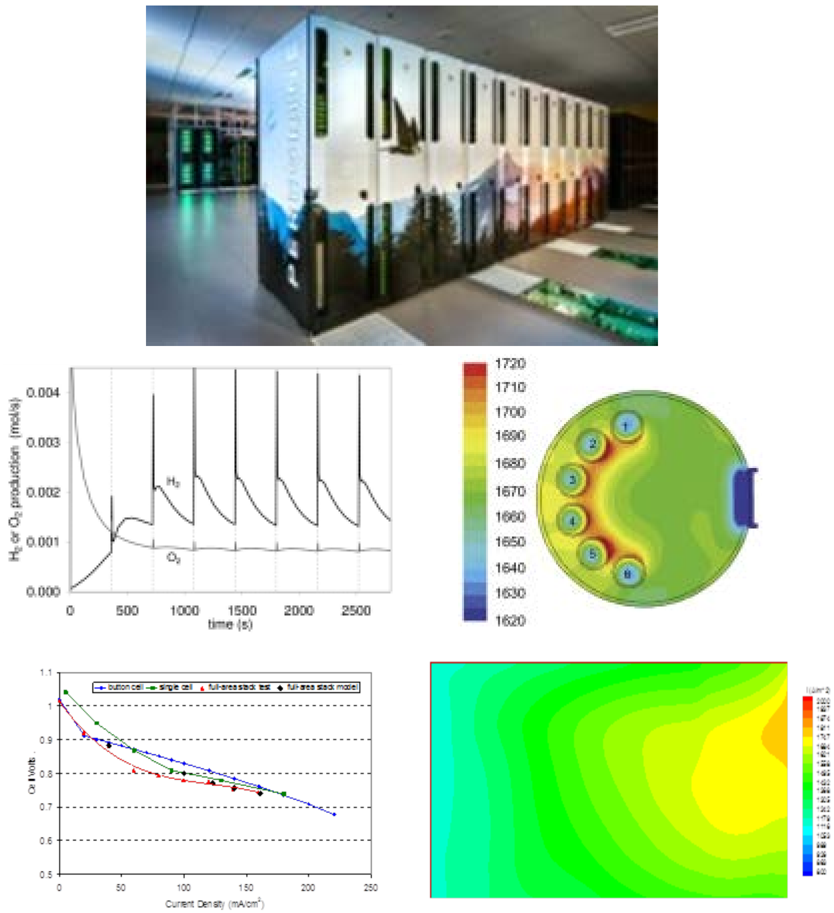
Purpose: The platform is a comprehensive computational tool for predicting solar to hydrogen (STH) efficiency of materials of known thermodynamic properties, under a wide range of thermochemical reactor design features and operating parameters and conditions.

Key Features:

- The rigorous accounting for all key aspects of two step thermochemical processes, allows for unsurpassed theoretical evaluation of candidate materials.
- The use of physical models that benchmark and standardize estimates STH efficiency given a sufficiently robust thermodynamic material model.

- “Efficiency Maximization in Solar Thermochemical Fuel Production: Challenging the Concept of Isothermal Water Splitting”, I. Ermanoski, J. E. Miller, M. D. Allendorf, Physical Chemistry Chemical Physics 16 (2014) 8418
- “Annual average efficiency of a solar-thermochemical reactor”, I. Ermanoski and N. P. Siegel, Energy Procedia 49 (2014) 1932

Multi-scale thermochemical and electrochemical modeling for material scale-up to component design

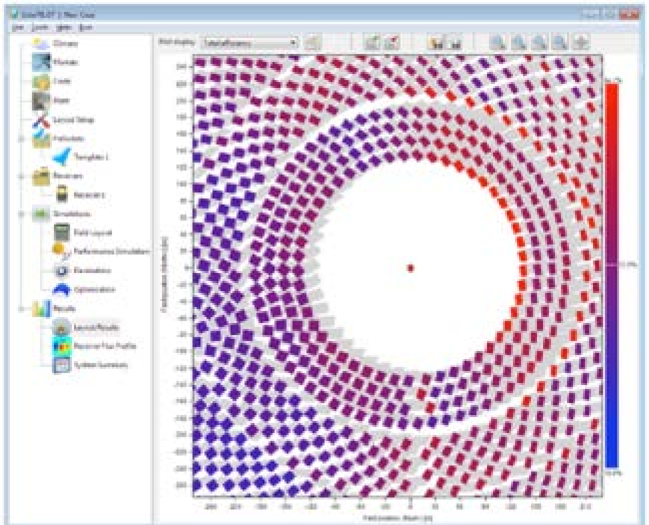


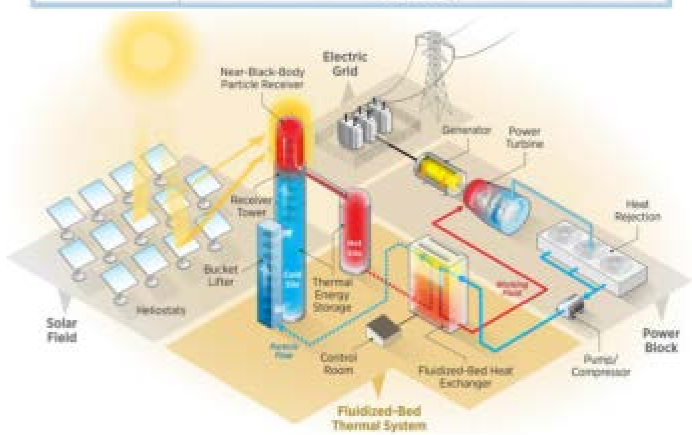
Purpose: This capability develops computational tools to **enable the implementation of materials into a component (STCH reactor) and to assess their performance, lifetime and reliability through high-fidelity modeling of a component design.**

Key Features:
- 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 to a solar thermochemical hydrogen process (STCH).

- 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.

Engineering of balance of plant (BOP) for high-temperature systems





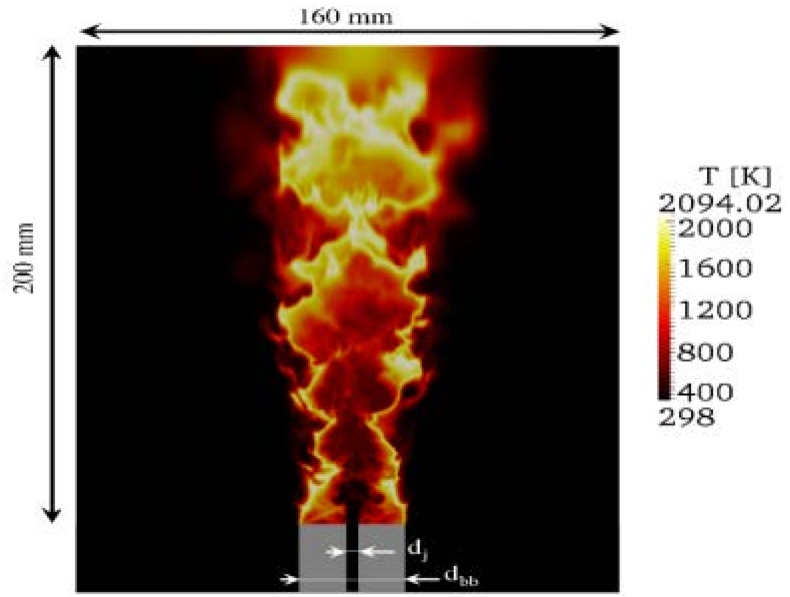
<u>Purpose:</u> This node serves the renewable integration of water splitting materials with engineering design of BOP for high-temperature electrolysis or STCH process.

<u>Key Features</u>:

- 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.

- 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.

Uncertainty quantification tool kit (UQTk) in computational models of physical systems



Large eddy simulations of turbulent combustion in a bluff body burner. UQTk was used for forward propagation of uncertainty in this system accounting for uncertainty in subgrid model parameters.

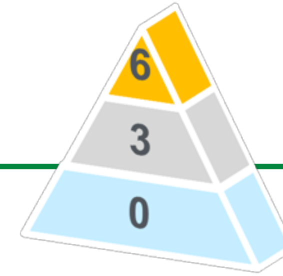
Purpose: To enable assessment of uncertainty in system predictions, thereby providing means for robust design optimization, qualification of design performance, and means for the use of predictions for decision support.

Key Features:

- UQTk offers methods for propagating input uncertainties through computational models, for sensitivity analysis, and for Bayesian calibration and parameter estimation based on experimental data.
- UQ methods have maximal utility when dealing with uncertain models and sparse/noisy data. They provide well-founded means for handling heterogeneous data from different experiments, observables, and scales; for estimation of model error in fitted models; comparing and selecting among models given available evidence; system/plant optimization under uncertainty, and making predictions with quantified uncertainty.

- A.C. Robinson, R.D. Berry, J.H. Carpenter, B. Debusschere, R.R. Drake, A.E. Mattsson, and W.J. Rider, “Fundamental issues in the representation and propagation of uncertain equation of state information in shock hydrodynamics”, Computers & Fluids, 83: 187-193, 2013.
- M. Khalil, G. Lacaze, J.C. Oefelein, and H.N. Najm, “Uncertainty Quantification in LES of a Turbulent Bluff-body Stabilized Flame”, Proc. Comb. Inst., 35:1147-1156, 2015

Synthesis/Process Capabilities



1. High flux solar furnace
2. Cascading pressure receiver reactor
3. National Solar Thermal Test Facility
4. Concentrating solar furnace
5. Spray pyrolysis
6. Membrane separators for hydrogen production

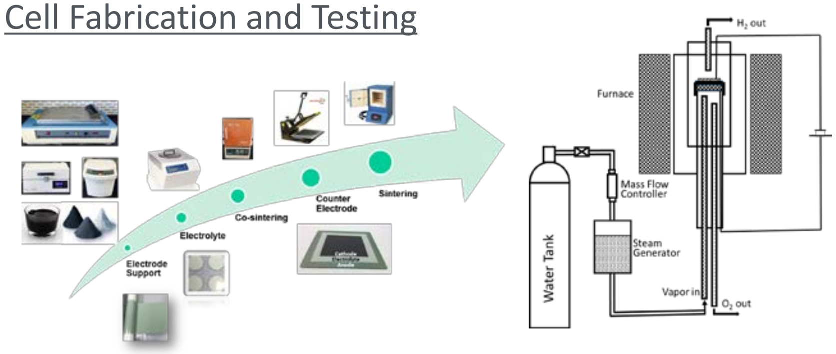
1. Advanced materials for water electrolysis
2. High throughput thin film combinatorial capability
3. Multiple Length scale additive manufacturing

CSP testing facilities, alternative synthesis methods, high-throughput combinatorial, acid electrolysis membranes

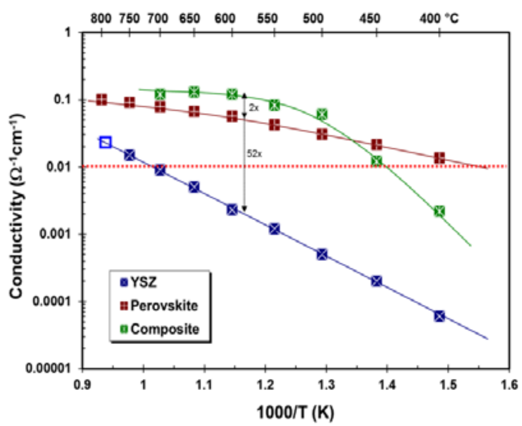
Note that many capabilities span different classification areas

Advanced materials for water electrolysis at elevated temperatures

Cell Fabrication and Testing



Advanced Electrolyte and Electrodes



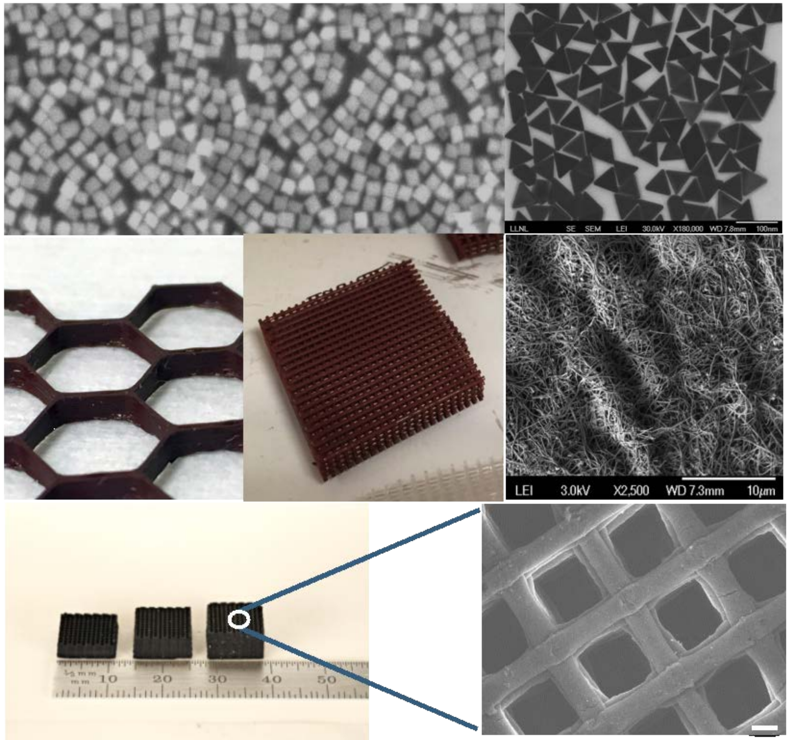
Purpose: This node focuses on the development of advanced electrode and electrolyte materials for water electrolysis at intermediate temperatures (200-600°C).

- 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

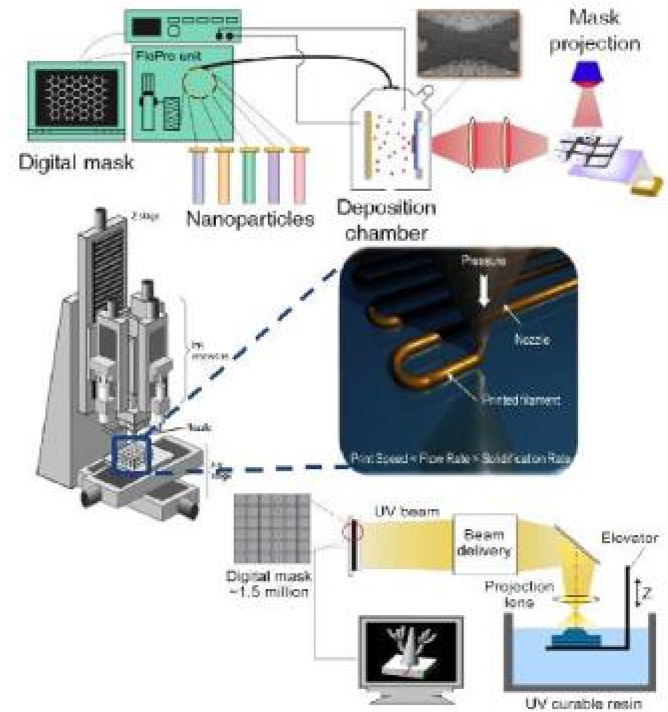
- Experts seek to improve ionic conductivity at intermediate temperatures by up to two orders of magnitude
- Lower operation temperature can reduce the chemical diffusion, migration, solid state reaction, corrosion, etc.
- Dry hydrogen, purification is not required
- Potential to eliminate Ni-catalysts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

Fabrication of custom electrodes at multiple length scales using additive manufacturing



Custom Materials Synthesis

Scale-Up

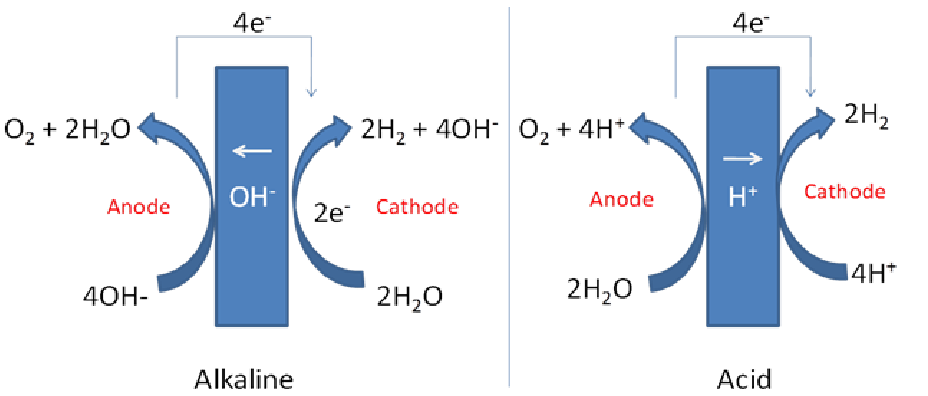


Additive Manufacturing

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.

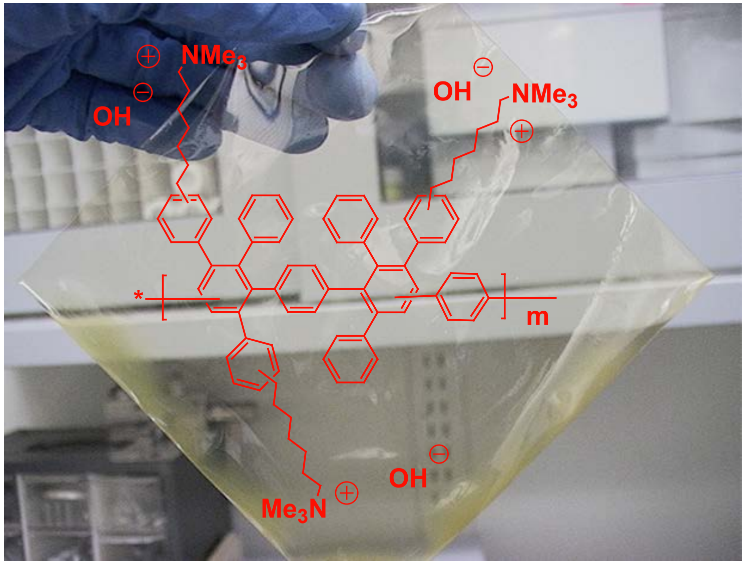
Separators for hydrogen production

Alkaline vs Acidic Electrolysis



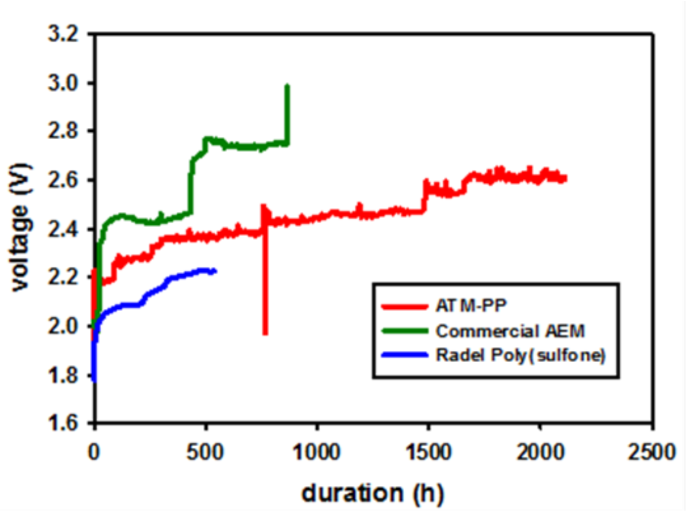
- Non precious metal catalysis
- Low cost separator

- Precious metal catalysis
- Nafion separator



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

+2000 h membrane performance



Chem Mater 26, 19 (2014) 5675-5682

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

High flux solar furnace (HFSF)

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:

- 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.

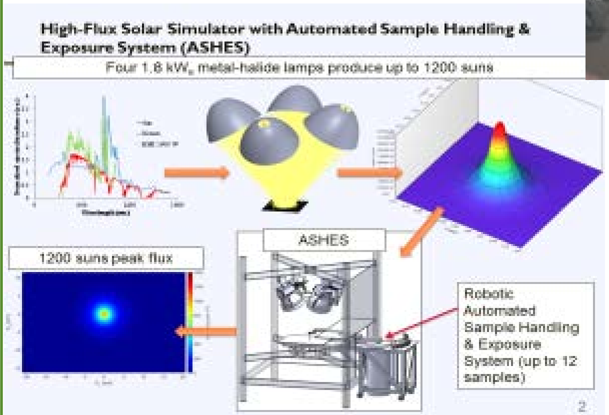
References:

- 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.

National Solar Thermal Test Facility (NSTTF)

16kW
solar furnace

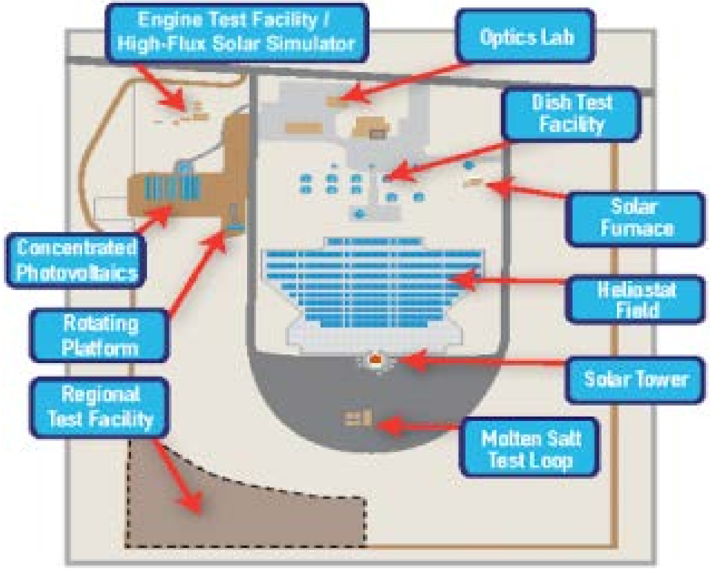
High-flux solar simulator



6 MW
power tower

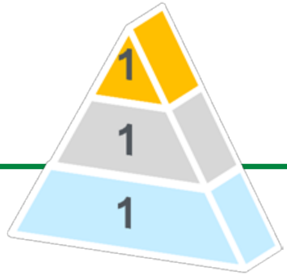
<u>Key Features</u>:

- 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/

Analysis Capabilities



1. TEA of hydrogen production

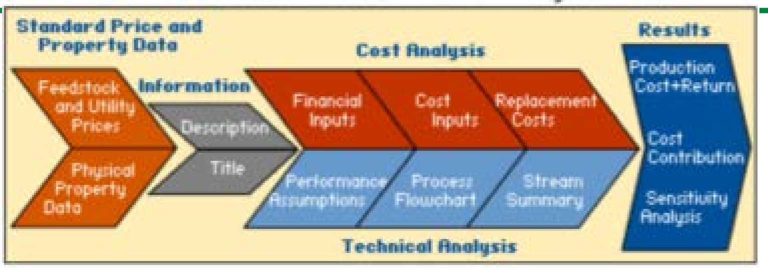
1. AWSM requirements based on flow sheet development and TEA

1. Prospective LCA modeling of hydrogen plant

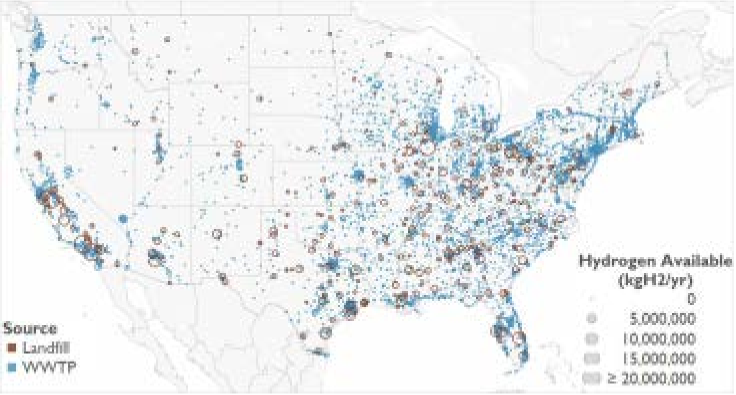
Note that most if not all projects will utilize these nodes

Technoeconomic analysis (TEA) of hydrogen production

H2A Production Cash Flow Analysis Tool

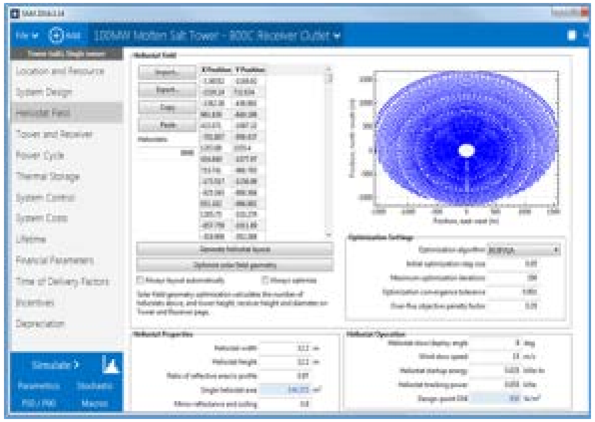


- Hydrogen Analysis (H2A) models
  - Production, Delivery, and Fuel Cells
  - Discounted cash flow framework
  - Models are transparent and public
    http://www.hydrogen.energy.gov/h2a_analysis.html



- 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

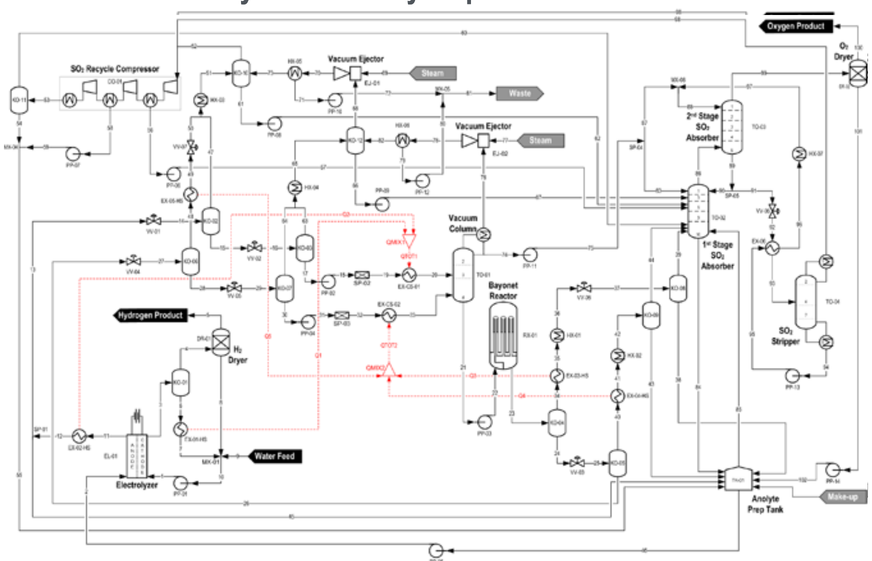
- NREL System Advisory Model (SAM)
  - Renewable resources including solar, wind, geothermal.
  - Economic and generation capacity models for planning
  - https://sam.nrel.gov/



- 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 TEA

Hybrid sulfur cycle process model

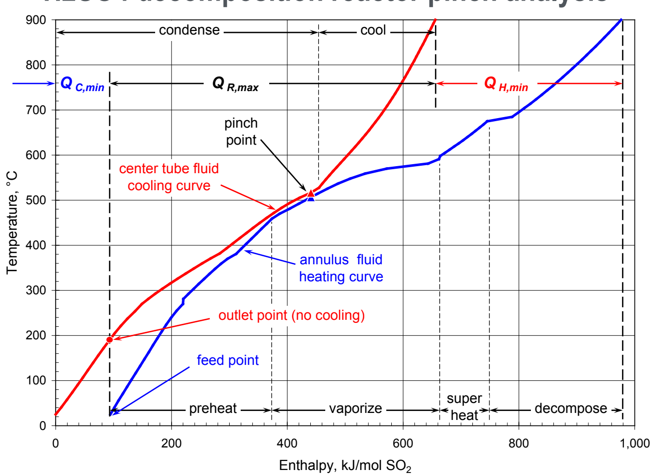


Unique capability for high-temperature water-splitting process development, modeling, and simulation

- 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

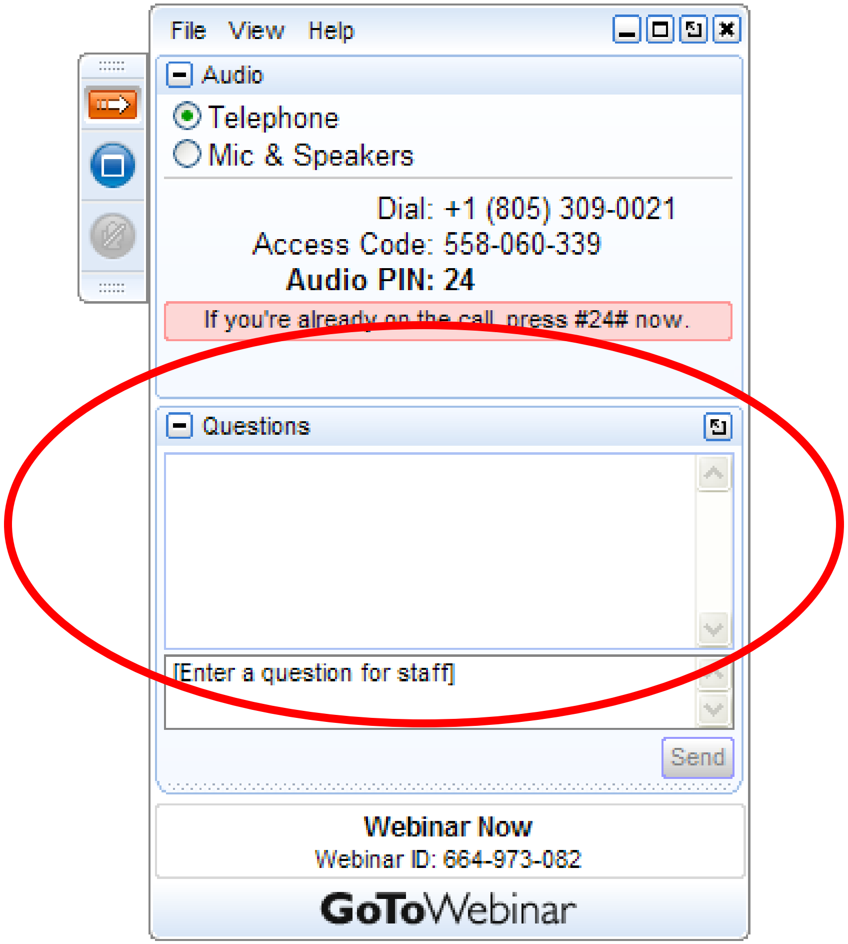
Webinars on HydroGEN EMN Consortia

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/121390860037074948	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/398336948352956164	Thursday, November 17th, 2016; 4 – 5 PM EST

Eric Miller, DOE-EERE-FCTO

Question and Answer

- Please type your questions into the question box



37

Thank you

Ben Klahr
(Benjamin.Klahr@ee.doe.gov)

Anthony McDaniel
(amcdani@sandia.gov)

hydrogenandfuelcells.energy.gov

List of STCH resource nodes

CLASSIFICATION	CATEGORY	RESOURCE NODE NAME	LAB
Characterization	2	TAPS, temporal analysis of products reactor system	INL
Characterization	1	In situ and operando testing using xrays	LBNL
Characterization	2	Surface analysis cluster tool	NREL
Characterization	2	Secondary Ion Mass Spectrometry (SIMS)	NREL
Characterization	3	Ex situ spatial characterization to support component integration	NREL
Characterization	3	Contamination Related capabilities	NREL
Characterization	3	Corrosion analysis of materials	NREL
Characterization	1	Advanced Electron Microscopy (FIB-TEM)	SNL
Characterization	1	High Temperature X-ray Diffraction	SNL
Characterization	1	Virtually accessible laser heated SFR for characterizing materials under extreme conditions	SNL
Characterization	3	Ambient pressure electrochemical XPS (E-XPS)	SNL
Characterization	1	High temperature catalyst and electrolyzer	SRNL

CLASSIFICATION	CATEGORY	RESOURCE NODE NAME	LAB
Computation	3	DFT and Ab Initio calculations for WS including real-time time-dependent DFT	LBNL
Computation	3	Multiscale modeling of WS devices	LBNL
Computation	2	Computational materials diagnostics and optimization of PEC devices	LLNL
Computation	3	Mesoscale kinetic modeling of WS and corrosion	LLNL
Computation	1	Multi-scale Thermochemical and Electrochemical modeling	NREL
Computation	1	Computational and Experimental Tools for enhanced STCH	NREL
Computation	2	First Principles Materials Theory for AWSM	NREL
Computation	2	Engineering BOP for High temperature systems	NREL
Computation	1	Albany multiphysics research platform	SNL
Computation	1	LAMMPS: Molecular dyanmics code for simulations of chemical and physical material processes	SNL
Computation	1	Uncertainty quantification in computational models of physical systems	SNL
Computation	2	Socorro: code for highly scalable DFT of extended systems	SNL
Computation	2	STH Efficiency Prediction platform	SNL
Computation	3	MOAB: Particle based mesh-free code for modeling transport and topological changes in liquids	SNL

List of STCH resource nodes

CLASSIFICATION	CATEGORY	RESOURCE NODE NAME	LAB
Analysis	3	Prospective LCA modeling of hydrogen plant	LBNL
Analysis	1	TEA of hydrogen production	NREL
Analysis	2	AWSM requirements based on flow sheet development and TEA	SRNL

CLASSIFICATION	CATEGORY	RESOURCE NODE NAME	LAB
Synthesis	2	Advanced materials for water electrolysis	INL
Synthesis	1	Spray pyrolysis	LBNL
Synthesis	2	Clean room and surface preparation	LBNL
Synthesis	2	Multiple Length scale additive manufacturing	LLNL
Synthesis	2	High throughput thin film combinatorial capability	NREL
Synthesis	1	Membrane Separators for hydrogen production	SNL

CLASSIFICATION	CATEGORY	RESOURCE NODE NAME	LAB
Process	1	High Flux Solar Furnace	NREL
Process	1	Cascading pressure receiver reactor platform	SNL
Process	1	National Solar Thermal Test Facility	SNL
Process	1	Concentrating Solar Furnace	SNL