



## COMPETITOR DIGEST

### Voucher Capabilities Menu

#### SELECT NATIONAL LAB HYDROGEN POWER CAPABILITIES

While this is not an exhaustive list, it is intended to help you determine the capabilities of labs that you could work with as a winning team of the Hydrogen Shot Incubator Prize.

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## Savannah River National Laboratory (SRNL)

Voucher Representative: [Charles James](#) & [Prabhu Ganesan](#)

### **High temperature corrosion, corrosion mitigation, and materials durability improvement for hydrogen production**

This capability consists of characterizing corrosion in high temperature systems and identifying methods to mitigate corrosion in the high temperature systems such as molten chlorides and molten fluorides

### **In situ and ex situ characterization of electrocatalysts and membranes for hydrogen production**

This capability consists of ex situ and in situ testing and fabrication of electrocatalysts and membranes. The ex-situ portion of the capability includes thin film catalyst deposition, catalyst screening using a variety of electrochemical techniques

### **Non-destructive material characterization**

SRNL's has 225keV and 450 keV X-ray DR/CT (Digital Radiography/Computed Tomography) and commercial software capability (Volume Graphics VG Studio software suite) to perform non-destructive analysis of different materials including additive manufacturing parts

### **Additive manufacturing**

SRNL has E-beam Powder Bed Fusion 3D printing capability to print Ti64 and CoCr alloy parts having complex design

### **Electromagnetic (EM)-assisted catalysis**

SRNL has induction- and microwave-assisted catalysis capability for carrying out chemical reactions such as deconstruction of plastics into high value products, gas phase dehydrogenation of hydrocarbons, and heavy crude oil upgrade

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## Pacific Northwest National Laboratory (PNNL)

Voucher Representative: [Jamie Holladay](#)

### Solid Oxide Electrolyzer and Fuel Cells

PNNL's experience in solid oxide electrolysis cell (SOEC) and fuel cell (SOFC) technology and related high temperature electrochemical devices extends back to 1987 and has been documented in over 150 peer-reviewed technical papers and numerous patents. With over 30 staff working in SOEC and SOFC's, PNNL's experimental and modeling experience and capabilities in high temperature electrochemistry encompass all aspects of the technology, from materials development/characterization to design, fabrication, and testing of cells, stacks, and systems. In addition to performing work for the U.S. Department of Energy and other agencies, PNNL has collaborated successfully with a number of industrial developers.

PNNL's high temperature electrochemistry laboratories contain all the materials synthesis, processing, fabrication and testing equipment necessary to develop and test solid oxide electrolyzers, fuel cells, stacks, and complete power systems. We can manufacture powders, tapes, button cells, planar cells (up to 300cm<sup>2</sup>), tubular cells and complete stacks.

- **Experimental Capabilities:**
  - 70 button cell test stands,
  - 3 short and full stack test stands (up to 5kW)
  - 6 intermediate cell/stack test fixtures (5x5 cm)
  - Half-cell & full-cell testing; I-V, EIS; Simulated Syngas or Reformate; Impurities (Cr, S, Cl, P, Hg, As, Se, Sb, K, Na, Si, B, etc.)
  - In-operando SOFC Tests in XRD; High Temperature Environmental SEM/TEM; Seals Development and Evaluation
  - Electrochemical characterization tools
- **Modeling:** Proprietary and publicly available stack modeling (finite element analysis, computational fluid dynamics, ceramic analysis & reliability engineering software, mechanical stress, heat transfer and fluid flow analysis, electrochemical performance, structural reliability, micromechanics damage, fracture and failure modeling and more)
- **Fabrication:**
  - Fabrication techniques: Tape casting (5' & 8' casters); Screen printing; Compression molding; Injection molding; Tape calendaring; isostatic & uniaxial pressing; slip casting; extrusion; laser & e-beam welding; brazing; Controlled atmosphere sintering; Spinel coating and aluminization
  - Thin film techniques: Spin coating; PVD; E-beam; Sputtering; PLD; Slurry and solution coating; Spray coating
  - Materials synthesis: Glycine-nitrate combustion synthesis; Liquid & solid precursor techniques
- **Analysis and characterization (including stack post-mortem analysis):**
  - Microscopy: SEM/EDS/EBS/EDS; FIB/TEM; EPMA; OM
  - Spectroscopy: SIMS, Nano-SIMS, XPS, Auger, Raman, FTIR, NMR
  - Controlled Atmosphere Dilatometry; TGA/DSC
  - Electrical Conductivity/Seebeck; Hydrogen/Oxygen Permeation
  - Mechanical Properties (Strength, Hardness, Modulus); Surface Profilometry; Particle Size; BET Surface Area Analysis

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## Hydrogen Materials Compatibility

PNNL is a leader in hydrogen-polymer materials compatibility. PNNL co-leads the H-MAT consortia with Sandia National Laboratory. These capabilities are also used in support of the blended gas CRADA and composite overwrap pressure vessel. Pressure vessel work for new fiber systems, sizing interface, and cryogenic storage are supported under this capability. Some of our available capabilities include:

- PNNL has test frames in environmental chambers allowing testing from -129C to 315C
- Ex-Situ Polymer testing: hydrogen saturated cryogenic tests at -230C temperatures and up to 100 MPa pure hydrogen
- In situ tribometry - Friction and wear testing in H<sub>2</sub> atmosphere (38 MPa), PV range up to reciprocating compressor speeds and forces
- micro X-Ray CT for internal damage
- Blended gas materials evaluations
- High pressure observation cell to image material behavior in real time for swelling/pressure relationships
- Materials testing site flow system for pipe fracture mechanics in hydrogen and blends using real time crack propagation measurements
- Refueling hose burst pressure measurements from -130C to 300C, and up to 500 MPa burst pressure
- Pipe burst testing
- Pipe joint testing and leaking
- H<sub>2</sub> impact on materials before and after hydrogen exposure to look for correlations with other tests
  - Hardness changes – directly after exposure and 1 week after
  - Swelling – directly after exposure and 1 week after
  - Sensible with free volume and diffusion considerations
  - Crystallinity changes influenced by hydrogen
  - Fracture energy
  - Creep and slow crack growth
- Materials characterization
  - Dynamic mechanical analysis
  - DSC- Differential scanning calorimetry
  - Thermogravimetric analysis (TGA)
  - X-ray diffraction
  - Density
  - Thermal desorption spectroscopy
  - Permeation cell, -40C to 120C
  - Diffusion calculations
  - Material saturation concentrations per pressure
  - Composite material testing for pressure vessels
- Material compounding and fabrication
  - Rubber formulation development
  - Model material system development for evaluating material additives not hydrogen compatible
  - X-winder for small scale filament winding
  - Composite fabrication for material testing and evaluation



## Hydrogen Storage

PNNL has been engaged in the development of materials-based hydrogen storage for over 20 years, from 2005-2010 as part of the Chemical Hydrogen Storage Center of Excellence, from 2010-2015 as part of the Engineering Center of Excellence; from 2015-2018 as part of the Hydrogen and from 2018 to present as part of the Hydrogen Advanced Materials Research Consortium.

- **Characterization tools**
  - 20+ Nuclear Magnetic Resonance Spectrometers (NMR) for <sup>1</sup>H, <sup>2</sup>H, <sup>11</sup>B, <sup>13</sup>C, <sup>15</sup>N, <sup>19</sup>F, <sup>31</sup>P, <sup>27</sup>Al.
    - Variable pressure (atmospheric to 200 bar), variable temperature, 200 – 500 K solid state magic angle spinning (MAS) NMR
    - Dynamic nuclear polarization (DNP) for ultra-high sensitivity
    - Variable low temperature (4- 100 K) static NMR
    - Variable pressure (atmospheric to 100 bar) solution phase NMR
  - PNNL leads in the development and application of electron microscopy tools, including in situ electron microscopy.
- **Calorimetry**
  - Solid state and liquid phase reaction calorimetry (Calvet)
  - Differential scanning calorimetry (DSC) coupled with IR and mass spectrometry
  - Isothermal titration calorimetry.
- **Synthesis and characterization of molecular and heterogeneous catalysis**
  - Inert atmosphere capability for reactors
  - Hydrogenation and dehydrogenation capabilities coupled with spectroscopy to monitor kinetics of gas formation
  - Autoclave reactor banks (6 autoclaves) for variable temperature variable pressure kinetic studies
- **Multi-scale modeling**
  - NWChem code for quantum mechanical simulations of chemical properties of materials. It allows for extremely accurate calculations of properties relevant to hydrogen interaction with materials. NWChem also scales very well with the number of CPU nodes which makes it very attractive for running on DOE's high-performance computing facilities. To the best of my knowledge, PNNL is unique among DOE's national laboratories in having developed a code like this. Karol Kowalski leads the NWChem team.
  - Petr Sushko's expertise in quantum mechanical materials modelling. During the past decade he has worked on a number of problems including adsorption and reactivity of hydrogen on surfaces, dissociation of H<sub>2</sub> on surface defects, hydrogen diffusion and interconversion, and properties of disordered materials including rough surfaces, interfaces, amorphous silica, and solid solutions.
  - Sorbents modeling
    - De novo design of hierarchical sorbents with tuned molecular control of interactions with hydrogen
    - Integrated electronic structure simulation tools to predict structural building unit self-assembly in aqueous and non-aqueous solvent systems to enable practical synthesis routes for the materials
    - First principles design of new polymer-MOF sorbent materials to achieve high volumetric/gravimetric hydrogen storage density
  - Density functional theory studies of binding energies and transition states

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- Classical molecular dynamics simulations of dynamical processes, such as diffusion, defect interactions, and phase changes
- Monte Carlo studies of diffusion in complex hydrides with input from DFT
- Phase field modeling of microstructural evolution, amorphous regions etc. at different temperatures
- COMSOL multi-physics simulations of hydrogen flow, thermal conductivity etc.
- **Materials**
  - Sorbents development- have fabrication facilities for nano-materials and fully capable to manufacture MOFs and other nano-materials from the sub-gram to 100's of gram levels.
  - We have experience scaling up manufacturing processes.
  - Custom built Sievert's system flexible for low or high pressure measurements
  - PCT-Pro (Setaram)
  - Custom built thermal conductivity device for <1 kg beds
  - Laser Flash for thermal conductivity measurements
  - TGA/DSC/MS
  - Calorimetry
  - BET surface analysis
  - Multiple ball mills (low and high energy)
  - Glove boxes
  - Schlenk lines
  - XRD (powder and single crystal)
  - EMSL User facility: multiple NMRs and TEMs (including in situ); in situ XRD
  - Computational: DFT, MD, BOMD
- **Electric Grid** (<https://www.pnnl.gov/electric-grid-modernization>)
  - Hydrogen Energy Storage – HESET – (<https://www.pnnl.gov/news-media/hydrogen-energy-storage-your-service> and <https://eset.pnnl.gov/overview?next=%2F>) The Energy Storage Evaluation Tool (ESET) is a suite of modules and applications that utilities, regulators, vendors, and researchers can use to model, optimize, and evaluate various energy storage systems: **hydrogen**, pumped storage hydropower, microgrids, batteries, and thermal mass stored in buildings. The tool examines a broad range of use cases and grid applications to maximize energy storage system benefits from stacked value streams—multiple uses at the same time.
- **Distribution and transmission modeling analysis tools** (such as GridPack, Adaptive RAS/SPS, EMS 2.0, Dynamic Paradigm for Grid Operation, DCAT (including machine learning and AI), etc.)
- **Grid Architecture** - Grid Architecture is the application of system architecture, network theory, and control theory to the electric power grid. A grid architecture is the highest level description of the complete grid, and is a key tool to help understand and define the many complex interactions that exist in present and future grids. (<https://www.pnnl.gov/grid-architecture>)
- **Grid Cyber security** (<https://www.pnnl.gov/grid-cybersecurity>) - New cyber awareness strategies from PNNL is increasing the ability to share information about threats, vulnerabilities, and mitigation strategies with people who can put that information to work. Example capabilities include
  - Electricity Infrastructure Cybersecurity and Resilience Center at PNNL
  - The Power Networking, Equipment, and Technology Testbed (powerNET) is a remotely accessible, multi-user, experimental testbed to support power system and smart grid research.
  - Energy Communications Cyber Test Range, a software-defined radio test range with a two-mile-plus radio frequency range and more than six miles of optical fiber.
- **Solid Phase Processing and Joining** (<https://www.pnnl.gov/solid-phase-processing>) Solid phase processing (SPP) has the potential to significantly decrease the energy used in manufacturing. and deliver higher-performing components—all at a lower cost. SPP applies mechanical energy—in the form

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of high shear strain—to the metals to create friction heat for deformation. With SPP, metals are not melted, resulting in a significant decrease in the energy intensity of alloy and component manufacture. This process enables the microstructure of the metal to be tailored to yield superior properties.

- Friction stir welding and friction stir scribe (unique to PNNL)
- Shear Assisted Processing and Extrusion (unique to PNNL)
- Ultra-high velocity cold spray (unique to PNNL)

## Hydrogen Safety

For over two decades PNNL has been a leader in hydrogen safety. We have developed unique capabilities for the hydrogen community.

- **PNNL Hydrogen Safety Panel (HSP):** The PNNL HSP is an essential resource to address the concerns about hydrogen as a safe and sustainable energy carrier, using over 400 years of cumulative hydrogen safety experience, including committee members from National Fire Protection Association, Society of Automotive Engineers, American Society of Mechanical Engineers, and the International Standards Organization
- **Hydrogen Risk analysis:** PNNL uses their deep knowledge in risk analysis to evaluate and quantify the risks of hydrogen under various scenarios.
- **H2Tools:** a one-stop site for information on hydrogen safety, best practices, lessons learned and codes and standards
- **First Responder training (hands on and virtual):** PNNL has developed state of the art courses, including hands on training for first responders in an effort to “train the trainers”. We have developed First Responder Training Videos, classroom materials and field training

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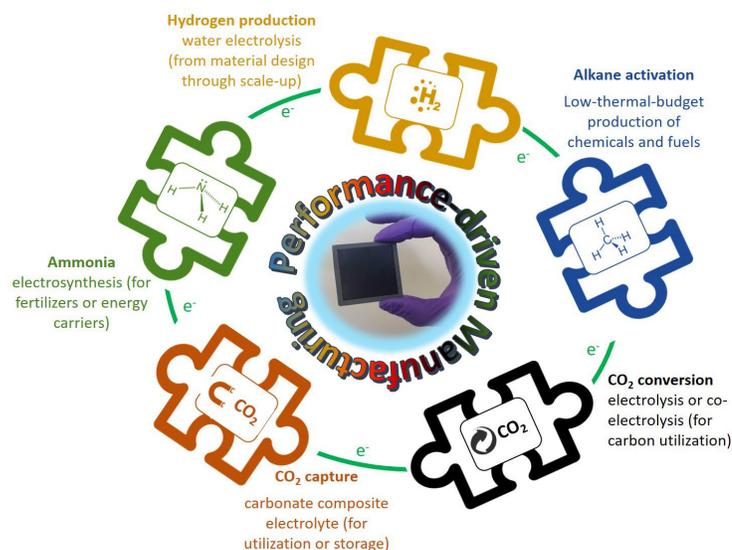
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## Idaho National Laboratory (INL)

Voucher Representative: [Dr. Dong Ding](#)

### The Electrochemical Processing and Electrocatalysis (EPEC) Lab

As a premier lab who holds the leadership in high temperature electrochemistry and solid oxide electrochemical cells, INL established a world-class program in electrochemical reactions at elevated temperatures (350-850°C) using unique solid oxide electrochemical cells (SOEC)/membrane reactors. Elevated temperatures drive electrochemical process efficiency. The primary research interests of the EPEC lab include fundamental understanding of the effect of structure, composition, morphology, and defects on electrical, chemical, catalytic, and electrochemical properties of ionic and electronic conductors, especially charge and mass transfer along surfaces, across interfaces, and through complex electrodes. Specifically, the team led by Dr. Dong Ding are focusing on developing new strategies, novel materials/structures and new processes for efficient and cost-effective chemical and energy transformation. Their research portfolio covers electrochemical conversion of inexpensive feedstocks to value-added chemicals, fuels and hydrogen, as well as relevant manufacturing and scaling-up techniques with reduced process energy and carbon intensity. The team demonstrated a series of processes with high yield and efficiency including:



*The research portfolio for the INL's electrochemical processing and electrocatalysis group.*

- Hydrogen production via water electrolysis (from materials design to scale-up)
- Production of chemicals and fuels via low-thermal-budget alkane activation (e.g. ethane, methane, propane and butane as the feedstock to co-produce olefin and hydrogen)
- CO<sub>2</sub> capture using a carbonate composite electrolyte (for utilization or storage)
- CO<sub>2</sub> conversion via electrolysis or co-electrolysis with steam (with high selectivity of CO/CH<sub>4</sub> or ethylene)
- Ammonia electrosynthesis (for fertilizers or energy carriers)
- Solid oxide fuel cells and direct carbon fuel cells (for power generation)

The work has been published in leading journals (e.g. Nature, Nature Catalysis, Nature Communications, Energy & Environmental Science, Advanced Materials, etc.) protected relevant intellectual property. These projects leverage a set of unique capabilities including advanced synthesis and bulk supply of powders, high temperature roll-to-roll (HT-R2R) manufacturing and additive manufacturing of electrochemical cells/stacks, high throughput material testing, elevated temperature electrocatalysis, and electrode engineering and

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diagnosis, etc (see details below). In particular, the team has special research emphasis on performance-driven advanced manufacturing with quality control and quality assurance. The lab can fabricate from small button cells for fundamental study, large format cells (e.g. 10 x 10 cm<sup>2</sup>), to the stack as prototype demonstration. The capability also includes a wide range of high-temperature electrolysis (HTE) test facilities at difference scales including button cells, large format single cells, short stack and large stack etc., providing fast feedback for manufacturing and operation optimization. The research team has become a national lab example that is cable of not only transferring scientific knowledge to applied technologies by themselves readily but can bridge the gaps between academia and industry by promptly adopting innovations of the materials/structures developed by the former and providing the scaling-up experience/recommendations to the latter.



*INL's HT R2R and SOAM capabilities*

- **High temperature roll-to-roll (HT-R2R) manufacturing of electrochemical cells/stacks.** This capability allows us to fabricate systems from small button cells for fundamental studies through 10 cm x 10 cm planar cells, the industrial stack standard. This capability uses a conventional tape casting technique along with a lamination process by putting multi-green-tapes together. This capability can bridge the gaps between fundamental research and industrial deployment by guiding scale-up. In addition to the cells, the capability provides the inks, pastes, green tapes and laminates for desired compositions and configurations. With the industrial scale laser cutter, the cell shape and configuration can be trim to meet the varied needs for the stack assembly.
- **Solid oxide additive manufacturing.** Similar to HT-R2R, the capability starts with a tape casting process to make an electrode support that serves as the substrate for the layer-by-layer coating. A continuous inkjet printing process is applied to coat functional layer, electrolyte layer and subsequent electrode layer. The unique coating technology can deposit the layer as thin as 2-3 um with good homogeneity. It can also facilitate the surface modification of the electrode via catalyst coating, thus enhancing the performance and lifetime.

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## High Throughput Material Testing (HTMT)

- Thirty electrochemical testing stands for button cells, and 8 testing kilns for large format cells/short stack, equipped with multi-channel testing fixture/reactors to meet varied testing conditions and requirements, which can be coupled with multi-channel electrochemical work stations (independent potentiostat and frequency response analyzers), electronic load and power supply, along with cutting-edge gas chromatography and mass spectrometer for online qualitative and quantitative characterizations. It is powerful for quick materials screening and selection, enabling prompt material/catalyst R&D.

## Advanced synthesis and bulk supply of powders

Advanced synthesis and bulk supply of powders embraces a variety of methods to synthesize oxide raw powders in order to achieve controlled particle size, distribution and morphology for desired properties, include but not limited to solid state reaction, co-precipitation, sol-gel, and nitrite-combustion etc. Well-equipped bench-scale to production scale facilities enable the bulk supply of these powders up to 5 kg in one batch with reproducible performance for scale-up needs, facilitated by particle analyzer, surface area analysis, and chemical and thermal expansion measurement in a controlled gas atmosphere.



## Supply chain for manufacturing of solid oxide electrochemical cells

Electrode Engineering and Diagnosis can manipulate the microstructure and porosity of the electrode by tuning pore formation or integrating novel 3D electrode architectures. Electrocatalysts coating can be introduced subsequently through wet infiltration, hydrothermal deposition or atomic layer deposition. The surface coating may consist of discrete particles, or a continuous thin film. These modifications can serve as a new functioning layer, effectively utilizing the unique properties of two different materials and thus offering multi-functionality. It can also study the microstructural evolution, relating to the performance change by both experimental observation and simulation including tomography, CT-scan, 3D reconstruction, density functional theory, phase field theory, multi-physics, and uncertainty models.

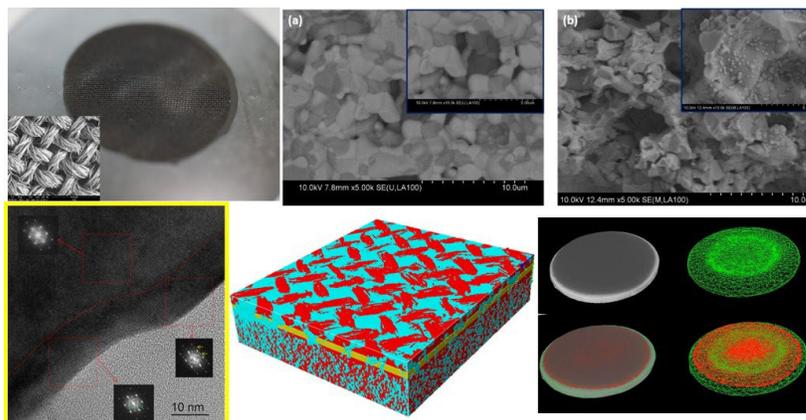


*INL's capability of supply chain for manufacturing of solid oxide electrochemical cells.*

## Electrode engineering diagnosis for solid oxide electrochemical cells

The Elevated Temperature Electro catalysis platform consists of the electrochemical testing stands and a series of specially designed reactors that can integrate solid catalyst materials with electrochemical cells to conduct electrocatalysis measurements under elevated temperatures and pressure conditions. A fully automated physisorption/chemisorption analyzer interfaced with on-line mass spectrometer for a range of characterizations include BET surface area/pore structure analysis, temperature programmed,

pulse chemisorption and physisorption analysis of dispersed catalyst materials. An operando Fourier-transform infrared spectroscopy (FTIR) is capable of IR spectroscopic studies of solid oxide electrochemical cells in a diffuse reflectance mode. It also includes thermal gravimetric analysis under extreme environment (e.g. high steam concentration), This capability enables to perform fundamental studies of catalytic materials for electrochemical processing.



*INL's capability of electrode engineering and diagnosis for solid oxide electrochemical cells.*

## Elevated temperature electrocatalysis



The capability layout and showcase of Elevated Temperature Electrocatalysis.

- **Large scale electrochemical testing:** INL has a long track record high temperature electrolysis (HTE) with test facilities at from small cells through a 250-kW system (under construction). The 25-kW HTE flexible test facility has capability of performance evaluation of SOEC stacks operating independently or in thermal integration with co-located systems. This is designed to demonstrate operation in a variable grid with thermal energy integration. It could be operated to produce H<sub>2</sub> in electrolysis or integrate with carbon utilization in co-electrolysis.



Overview of the 25-kW HTSE experiment skid and enclosure within the INL System Integration Laboratory.

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## Lawrence Berkeley National Laboratory (LBNL)

Voucher Representative: [Adam Weber](#)

LBNL works on hydrogen technologies across the make/move/store/use paradigm including integrated analysis and fundamental to applied research (<http://hydrogen.lbl.gov>).

### FlexLab

LBNL runs the FlexLab (<https://flexlab.lbl.gov/>), which is the world's most advanced integrated building testbed. This provides instrumented capabilities to plug and play various building-related technologies.

### Leadership

LBNL sits at the leadership level of several DOE consortia including co-Director of the Million Mile Fuel Cell Truck (M2FCT) Consortium for improving fuel cell durability and performance, Deputy Director of HydroGEN Energy Materials Network focused on advanced hydrogen generation technologies, HyMARC focused on novel materials storage concepts including carriers, sorbents, and hydrides, and Deputy Director of H2NEW consortium which is focused on high and low temperature electrolysis. Within these activities LBNL can supply:

- Single-cell solid-oxide and proton-conducting oxide cell testing and associated diagnostics including impedance
- Single-cell testing from 5 to 100 cm<sup>2</sup> for fuel cells and electrolyzers including proton and hydroxide conducting membrane technologies.
- Extensive component characterization capabilities ranging from transport and structural properties to behavior of integrated studies to beamline studies of key phenomena.
- Various fabrication techniques and procedures for making integrated assemblies of components including various ink characterization and deposition expertise.

### Other Capabilities

- LBNL has extensive experience in technoeconomic analysis and life-cycle assessment that has been utilized for different hydrogen technologies from production to deployment. LBNL also focuses on impact to local communities and takes a holistic approach of looking at energy return on energy investment for full scale deployment of hydrogen technologies. Analysis also includes DFMA.
- Physics-based modeling expertise across different scales and technology platforms from geologic hydrogen storage to cell performance and durability to ab-initio catalyst activity.

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## Argonne National Lab (Argonne)

Voucher Representative: [Amgad Elgowainy](#)

### Hydrogen Infrastructure Techno-economic Modeling and Analysis

- Argonne developed “pressure consolidation”, a patented smart-fueling technology, to reduce fuel-station equipment costs by 30%. The patent was licensed to PDC Machines, and funding was provided by EERE’s Technology Commercialization Fund (TCF) for commercial demonstration.
- Argonne will demonstrate the patented technology with Hyzon Motors, a supplier of hydrogen fuel cell-powered commercial vehicles, and PDC Machines, in a public fuel station near Argonne.
- Argonne developed a suite of hydrogen infrastructure models that are used globally by over 3000 companies to evaluate the economics hydrogen delivery and fueling options (available at <https://hdsam.es.anl.gov/>). These include:
  - **HDSAM** (Hydrogen Delivery Scenario Analysis Model): Offers detailed techno-economic analysis of hydrogen delivery cost to end use applications.
  - **HRSAM** (Hydrogen Refueling Station Analysis Model): Offers detailed techno-economic analysis of hydrogen refueling and interaction with light-duty fuel cell electric vehicles.
  - **HDRSAM** (Heavy-Duty Refueling Station Analysis Model): Offers detailed techno-economic analysis of hydrogen refueling and interaction with heavy-duty fuel cell electric trucks and rail applications.
  - **H2SCOPE** (Hydrogen Station Cost Optimization and Performance Evaluation) model: evaluates various fuel station and vehicle tank design options for lowest cost options while observing safe fueling of fuel cell vehicles.

### Environmental Life Cycle Analysis

- Argonne developed the GREET® model (available at <https://greet.es.anl.gov/>), which evaluates lifecycle carbon footprint for hydrogen production, delivery for various end use applications, and allows evaluation of the decarbonization potential of hydrogen production pathways.
- GREET will be used to guide DOE’s clean hydrogen standard (CHS) and the subsequent potential hydrogen production tax credits (PTC) if approved by congress.
- Argonne is contributing to the development of green hydrogen certification method under the International Partnership of Hydrogen Economy (IPHE)
- Argonne’s GREET model has been used to inform R&D directions and government actions such as:
  - California’s Low-Carbon Fuel Standard.
  - Canadian Clean Fuel Standard.
  - The International Civil Aviation Organization’s Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA).
  - International Partnership for Hydrogen and Fuel Cells (IPHE).
  - The International Hydrogen Infrastructure workshops.



## Additional Modeling

- Argonne pioneered and continues to lead Life Cycle Analysis (LCA) through GREET and its derivatives:
  - **VISION**: Estimates fleet impacts of highway vehicle technologies and fuels on energy use and greenhouse gas (GHG) emissions to 2050.
  - **NEAT** (Non-highway Energy and GHG emission Accounting Tool): Estimates impact of freight movement on energy and GHG emissions.
  - **AFLEET** (Alternative Fuel Life-cycle Environmental and Economic Transportation tool): Estimates energy, emissions, and costs of alternative fuel vehicles.
  - **Bioeconomy AGE** (Bioeconomy Air Emissions, Greenhouse Gas Emissions, and Energy Consumption): Estimates energy and emissions effects of bioenergy and bioproduct scale up.
- Techno-economic analysis (TEA) of hydrogen production, delivery and fueling, and production of synthetic fuels, ammonia and chemicals from renewable hydrogen and CO<sub>2</sub> sources using its HDSAM platform.
- Argonne has been supporting the DOE's EERE EEEJ roadmap working group through analysis of employment and equity impacts of technology development and deployment. Argonne's transportation energy burden analysis has been used by the DOE to identify disadvantaged communities and inform the recent BIL's NEVI Formula Program to determine underserved areas for the siting EVSE. Additionally, Argonne has been developing JOBS tools to evaluate the employment impacts of alternative fuel production and deployment, including hydrogen and electrification technologies.

## Enabling Fuel Cell Adoption

- Argonne innovations enabled by unique facilities – the Advanced Photon Source, Argonne Leadership Computing Facility, and Center for Transportation Research – improve cost, performance, and durability.
- Argonne is addressing fuel cell performance challenges on multiple fronts:
  - Catalyst development – high-activity platinum-based and PGM-free catalysts lower fuel cell cost.
  - Degradation– improved understanding of catalyst degradation increases durability and performance.
  - Modeling and characterization – optimization of fuel cell to improve performance and reduce cost.
  - Vehicle testing – evaluation of fuel cell vehicle performance under a wide range of conditions.
- **The Million Mile Fuel Cell Truck (M2FCT) Consortium**
  - Argonne is working with other national labs as part of the Hydrogen and Fuel Cell Technologies Office (HFTO) M2FCT consortium to improve the efficiency, durability and cost of fuel-cell systems.
  - M2FCT's goal is achieving an aggressive target for proton-exchange membrane fuel cells (PEMFC) heavy-duty vehicle (HDV) membrane-electrode assemblies (MEAs) that combines efficiency, durability, power density, and cost in a single metric.
  - Argonne holds two deputy director positions on the Steering Committee, leads two M2FCT tasks (Analysis and Materials Development), and contributes research to all M2FCT tasks.

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## Other Activities

- **H2NEW Consortium**
  - Argonne researchers are working with their counterparts at other national labs as part of the Hydrogen from Next-Generation Electrolyzers of Water ([H2NEW](#)) consortium.
  - The objective is to improve the performance and durability of electrolyzers, reduce the cost of producing clean hydrogen and achieve the Hydrogen Shot goal (\$1 per kilogram in one decade).
- **ElectroCat Consortium**
  - Argonne co-leads HFTO's Electrocatalysis ([ElectroCat](#)) consortium.
  - ElectroCat 2.0 targets development of platinum group metal (PGM)-free catalysts for (PEMFC) cathodes and for alkaline and proton exchange membrane electrolyzer anodes.
  - Goal is to develop catalysts for fuel cells and electrolyzers that use abundant, less-costly metals such as iron, cobalt, and nickel.
  - Argonne's research roles in ElectroCat are high-throughput synthesis, activity screening, and device performance evaluation of catalysts and the characterization of materials, electrodes, and devices.

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## Lawrence Livermore National Laboratory (LLNL)

Voucher Representative: [Brandon Wood](#)

### Systems

- **Cryogenic Hydrogen Test Facility:** Unique prototype testing facility for cycle testing at cryogenic temperatures with hydrogen. Features liquid hydrogen (LH2) technologies, including a 3,000 gallon LH2 Dewar, a 100 kg/hr cryopump capable of reaching high pressures (up to 875 bar) over a wide spectrum of temperatures (50 to 300 K), and a three cubic meter containment vessel in which cycle testing of non-certified parts can be carried out remotely with cryogenic hydrogen.
- **Energy Systems Site for Operations & Simulations (ESSOS):** Grid resiliency research and testing facility, with planned future expansion to hydrogen technologies. Used for testing and validation of integrated systems and components in a dynamic environment across a range of conditions using a cyber/physical, real-time computational platform.
- **North American Energy Resilience Model (NAERM):** Multi-lab effort to develop steady-state and transient gas pipeline models coupled with electric grid transmission models. Historically focused on natural gas, the models can be re-purposed to include hydrogen for exploration of future hydrogen pipeline strategies and the impact of outage on the electric grid.

### Materials & Manufacturing:

- **Laboratory for Energy Applications for the Future (LEAF):** Integrated simulation, characterization, and manufacturing capabilities for design of reactors and electrolyzer components, including foundational research efforts into performance and degradation of materials.
- **High-performance Computing for Energy Innovation (HPC4EI) and High-performance Computing Innovation Center (HPCIC):** Programs focusing on the application of high-performance computing to material- and device-level simulations for direct collaboration with industry, including hydrogen technologies.
- **Advanced Manufacturing Laboratory (AML), housing the Hydrogen Materials Laboratory (HML):** Facilities to test degradation of materials and components in hydrogen environments, as well as to demonstrate prototyping of optimized materials designs via 3D printing, laser processing, and other advanced manufacturing techniques.
- **HPC for DOE Hydrogen Consortia:** LLNL leads high-performance computing modeling and simulation efforts within three DOE hydrogen consortia: HydroGEN Advanced Water Splitting Materials (focused on emerging technologies for renewable hydrogen from water), Hydrogen Materials—Advanced Research Consortium (HyMARC, focused on materials-based hydrogen storage and carriers), H2NEW High-temperature Electrolysis (focused on degradation and manufacturing of steam electrolyzers).

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## National Renewable Energy Laboratory (NREL)

Voucher Representative: [Huyen Dinh](#)

### Techno-Economics Analysis (TEA)

NREL's hydrogen research includes TEA, specifically with regards to long-duration energy storage, blending hydrogen into natural gas pipelines, total cost of ownership for heavy-duty vehicles, and supply chain optimization modeling. NREL's modeling tools include:

- **H2A** – financial analysis framework for estimating the cost of production of hydrogen (<https://www.nrel.gov/hydrogen/h2a-production-models.html>).
- **H2FAST** – hydrogen financial analysis scenario tool. Flexible, but originally built for hydrogen refueling stations (<https://www.nrel.gov/hydrogen/h2fast.html>).
- **StoreFAST** – TEA of hydrogen storage technologies (<https://www.nrel.gov/storage/storefast.html>)
- **SERA** – supply chain optimization.
- **RODeO** – grid integrated; optimized hydrogen production, storage, and renewable energy utilization cost analysis (<https://doi.org/10.1016/j.joule.2019.07.006>).
- **T3CO** – transportation technology total cost of ownership (e.g., medium/heavy duty trucks), analyzed using established models and OEM specifications.
- **REopt** – technoeconomic decision support platform used to optimize the sizing and operation of energy systems (<https://reopt.nrel.gov/>).
- **ReEDS** – regional energy deployment systems model projects utility-scale power sector evolution for the contiguous US using a system-wide, least cost approach. (<https://www.nrel.gov/docs/fy21osti/78195.pdf>).
- **H2OPP** – H2 hybrid optimization and performance platform: optimize co-located, utility-scale hybrid plants for different markets.

### Electrolyzer Testing

Electrolyzer testing is important for the verification, validation, and demonstration of electrolyzers at various scales. It is also important to understand the integration and scale up challenges of the technologies. NREL's testing capabilities include:

- **Single cell:** 16 proton exchange membrane (PEM) and 6 alkaline electrolyzer test stations
- **Short stack:** PEM electrolyzer (5–25 kW); highly automated; cell voltage monitoring
- **Full stack:** PEM electrolyzer test capability up to 1 MW; power supply capabilities of 4,000 A DC and 250 V DC; high fidelity control and data collection; dynamic, integrated controls; cell voltage monitoring; integrated with modular balance of plant (BOP) system; dryer system allows for capture of hydrogen for use in other applications.



## Hydrogen Infrastructure Research Capabilities

- **Hydrogen fueling:** comprehensive high flow rate fueling model validated with experimental data for 10 kg/min average fueling rate. Heavy duty fueling protocol support, 70 MPa and -40°C fast fueling, station design and operations.
- **Operations:** Compression, storage management, precooling, safety controls, back-to-back and simultaneous fueling
- **Storage:** Low, medium, high pressure ground storage, on-board vehicle storage (light duty, heavy duty), Type I–IV storage vessels
- **Components:** Reliability of early market components: valves, breakaways, nozzles, hoses
- **Safety:** integrate safety research into codes and standards; quantify component performance and failures from the field and in the lab; verify, validate, and develop prototype sensors with high accuracy and low cost; develop and deploy sensors and safety systems for hydrogen purity, leak detection; connect users to safety requirements to advance safe deployment.

## Hydrogen System Integration at Advanced Research on Integrated Energy System (AIRES) Platform

AIRES is a unique research platform designed to de-risk, optimize, and secure current energy systems and to provide insight into the design and operation of future energy systems at scale. The hydrogen system will enable both large-scale hydrogen systems R&D and broader energy systems R&D in alignment with H2@Scale vision.

- Integrated megawatt scale hydrogen production, storage, and fuel cell system at NREL Flatirons Campus consists of 1.25 MW PEM electrolysis (capability for up to two 1.25 MW electrolyzer stacks), 3,000 psi hydrogen compression, 600 kg ground hydrogen storage, 1 MW PEM fuel cell, power supply, power conversion, cooling system, water supply; dryer system allows for capture of hydrogen for use in other applications; direct electrical integration with solar and wind energy generation; capability to integrate with other large hydrogen assets.
- Energy systems control and optimization with electrolysis, storage, and end use considerations.

## Data Collection and Analysis

- Independent, secure management and processing of proprietary data
- Data from experiments, partners, inputs to models, BOP data are securely collected, stored, and analyzed to produce
  - Detailed data products: private, individualized results to support equipment and scalable models, and
  - Composite data products: publishable aggregated data to show status and progress, durability and efficiency, and can identify challenges.



## Stanford Linear Accelerator Center (SLAC)

Voucher Representatives: [Nicholas Strange](#) & [Xueli \(Sherry\) Zheng](#)

### Operando X-Ray Chemical Characterization of Low Temperature Electrolyzers (SSRL)

- A suite of X-ray characterization techniques enable studies under actual operating conditions via optimized *operando* cells.
- High-resolution X-ray spectroscopy tools to follow the chemical state of anode/cathode catalysts within electrolyzers. *Sensitive to: 1) chemical bonding, 2) reaction surface adsorbates, and 3) nanoparticle agglomeration*
- A recently developed advanced modulation-excitation approach enables isolating surface information from the bulk contribution that typically drowns the surface response when engaging conventional acquisition modes.
- Follow short and long-term performance degradation of devices
- Associate performance degradation with liquid products in electrolytes using online HPLC analysis and periodic electrolyte sampling for ICPMS – also ex-situ TEM imaging of catalysts.

### Synchrotron X-Ray Characterization of Materials and Devices for High Temperature Electrolysis (HTE) under operating conditions (SSRL)

- High-throughput diagnostic structural characterization (XRD) of aged high temperature electrolysis cells with simultaneous X-ray fluorescence for elemental analysis
- *In situ* (controlled temperature, flow, gas composition, electrochemical cycling) X-ray scattering and spectroscopy for identifying and differentiating degradation mechanisms in cell components
- Transmission X-ray microscopy for identifying microstructural changes to electrolyzer cells with 30 nm spatial resolution
- Spectro-chemical X-ray imaging with high-throughput X-ray absorption mapping instrument - enables understanding of heterogeneous structure and degradation with few-micron spatial resolution *in situ* (HTE & LTE).

### Photocatalytic production of H<sub>2</sub> (SSRL)

- Photocatalytic reactors and overall capabilities for characterizing absolute performance of photocatalysts under solar simulators and monochromatized light sources.
- Gas/liquid products quantification using online HPLC and micro-GC/RT-Mass Spectrometry
- X-ray characterization of photocatalytic materials under static illumination condition and upon laser pump x-ray probe time resolved approaches following the photocarriers dynamics.



## Evaluation of electrolyzer electrodes performance (SSRL)

- Benchtop stations for PEM/AEM electrolyzers and three electrodes flow cells (Biologic SP-300 potentiostats)
- Optimized quantification of gas production rates (HER/OER) using real-time mass spectroscopy (Diablo 5000B Real-Time Gas Analyzer - optimized down to  $\sim$ umol/hr online rates of H<sub>2</sub>) and micro gas chromatography (Agilent 990).
- Absolute faradaic efficiency and short- to long-term (months) performance evaluation for currents up to several  $\sim$ A/cm<sup>2</sup>
- Capabilities extend beyond hydrogen (e.g. CO<sub>2</sub>, NH<sub>3</sub>)

## Electrode synthesis (SUNCAT)

- Tools and capabilities to fabricate catalysts for gas diffusion electrodes or fundamental testing in a 3-electrode cell and integration of novel catalysts into electrolyzer architectures, including nanoscale and low precious metal content catalyst materials.
  - Physical Vapor Deposition System, Advanced Wet Chemical Syntheses Equipment, Ultrasonic Spraycoater, Hot/Cold Press

## Catalyst operando/in situ characterization (SUNCAT)

- Expertise in *in situ* characterization of hydrogen evolution and water oxidation electrocatalysts
  - Biologic Potentiostats (10 + channels), On-line Inductively Coupled Plasma-Mass Spectrometer (ICP-MS), Surface enhanced infra-red absorption spectroscopy (SEIRAS)

## Product analysis (SUNCAT)

- Characterization of product outflows online using gas chromatography to confirm H<sub>2</sub> and O<sub>2</sub> purity over time.
  - Electrochemical mass spectrometer

## Bench-scale electrolyzer performance and stability testing (SUNCAT)

- Instrumentation to test prototype electrolyzers at up to 10 A with device temperature and water flow control. Includes instrumentation to monitor for metallic component degradation
  - Electrolyzer Test Stations (2x)

## Density functional theory calculations

- Guided materials selection for hydrogen generation.



## National Energy Technology Laboratory (NETL)

Voucher Representative: [Nathan Weiland](#)

### NETL Capabilities Can Contribute to Successful Hydrogen Breakthroughs

The National Energy Technology Laboratory (NETL) has established significant capabilities that may be leveraged to help accelerate breakthroughs in clean and affordable hydrogen production technologies with the H-Prize: Hydrogen Shot Incubator. NETL can be a credible resource across a wide range of production configurations and in supporting the novel concepts your team is progressing to reduce the cost of hydrogen, particularly those derived from fossil-based resources.

**NETL offers analytical and assessment capabilities** with strategic systems analysis and engineering hosting over 140 scientists and staff to evaluate and de-risk system designs and provide systematic decision-making techniques that aim to balance the competing goals of costs and decarbonization.

**Technology Assessments include [Life Cycle Analyses \(LCA\)](#) and [Techno-Economic Analyses \(TEA\)](#)** to evaluate the performance, cost, and environmental emissions of demonstrated technologies and their supply chain.

- Extensive experience in applying comprehensive, rigorous, transparent methodologies to estimate the performance and cost of state-of-the-art technologies for hydrogen production from fossil-based resources with carbon capture. NETL recently completed a [comprehensive baseline study](#), of the cost, performance, and life cycle greenhouse gas (GHG) emissions of six hydrogen production technologies, *and* a [screening study](#) of other natural gas-fueled pathways to achieving the Hydrogen Shot goal.
- Developed and hosts the [LCA of the Natural Gas Supply Chain](#) to help minimize upstream GHG emissions from hydrogen production feedstock by evaluating over 120 natural gas basins and delivery routes, *and* supports the [Open Hydrogen Initiative](#) to assess and analyze the carbon intensity of hydrogen production.
- NETL's TEA focuses on plant technologies and their integration into energy markets along with core capabilities in steady state process design engineering and modeling (Aspen Plus®), full supply chain cost estimation and process system cost/performance comparative and tradeoff analysis.

NETL's **research and demonstration capabilities** can help validate hydrogen production technology considerations with our five-decades of study devoted to the conversion of fuels into higher-value products via various feedstocks, and carbon capture and subsurface management. NETL facilities, infrastructure, and capabilities can underpin the commercial scale up and demonstration of H<sub>2</sub> innovations.

1. **Optimal knowledge of H<sub>2</sub> subsurface potential with NETL leading the DOE National Laboratory [SHASTA project](#) for viability of subsurface hydrogen storage in unconventional formations.**
  - a. Leverages capabilities to quantitatively assess and manage long-term environmental risks of geologic CO<sub>2</sub> storage, and the adaptation to the technical aspects of hydrogen storage in salt, saline and depleted well formations



- b. Hydrogen impacts on well, reservoir, and caprock materials and geomechanics to examine the mechanical integrity of the wellbore, reservoir rock, and sealing rock with 410 unique field and reservoir combinations assessments.
- c. In-situ optical fiber sensors for real-time monitoring of parameters for hydrogen, methane and chemicals.
- d. Characterization of microbial communities with novel procedures to analyze complex hydrocarbon fluids and potential for hydrogen consumption.

**2. Support the commercialization of new technologies that are ready for demonstration.** In fuel conversions, feedstock validation, and testing, NETL knowledge resides in the conversion of natural gas, syngas, biomass, and/or waste plastic feedstocks to hydrogen and other products.

- a. Catalytic- and microwave-based methane pyrolysis processes for hydrogen production, as well as solid carbon product purification techniques.
- b. Microwave fundamental understanding, catalysts and interactions with scaling for hydrogen production through our [Center for Microwave Chemistry](#).
- c. Solid oxide electrolysis cells (SOEC) and solid oxide fuel cells (SOFC) to produce and use hydrogen, as well as modeling and experimental validation of performance and longevity.
- d. Structural materials expertise for hydrogen service and for high temperature and pressure applications, as well as considerable work in functional materials for catalysts, sensors, and gas separations. Specialty resides in supporting reduced embrittlement by designing microstructures, coatings and liners, alloy performance and assessing high temperature hydrogen attacks on steel and weldments, along with alloy development for improved hydrogen resistance.
- e. Sensor deployment with high sensitivity and selectivity, addressing ambient and harsh environments. This includes high temperature combustion sensing, low-cost fiber optic sensor array for simultaneous detection of multiple parameters, passive wireless sensors and electrochemical sensors.

**3. Testing and validation facilities and expertise**

- a. Geomechanics laboratories and capabilities to replicate and analyze engineered processes occurring at high pressure and high temperature conditions in the subsurface.
- b. NETL state-of-the-art Reaction Analysis & Chemical Transformation (ReACT) laboratory with developed and demonstrated microwave applications and high-pressure microwave reactor.
- c. Lab scale gasification test facilities, including TGAs, drop tube reactors, microwave gasification reactors, and small pilot test facilities. Expertise in refractory development for gasification environments, tar and syngas cleanup, and open source tools for multi-phase flow process [modeling](#) and [operability/optimization](#) of integrated energy systems.
- d. Design, modeling, and component testing for novel power and energy processes, including energy storage, supercritical CO<sub>2</sub> power cycles, chemical looping, etc., as well as carbon capture and utilization processes.

NETL is the only Government Owned-Government Operated (GOGO) laboratory in the Department of Energy (DOE) laboratory system with research and development (R&D) campuses located in Morgantown, West Virginia; Albany, Oregon; and Pittsburgh, Pennsylvania.

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## Los Alamos National Laboratory

Voucher Representative: [Rodney Borup](#)

The U.S. Department of Energy (DOE) awarded the first Fuel Cells for Transportation program to Los Alamos in 1977, eventually leading to what is now the DOE Hydrogen and Fuel Cell Technologies Office (HFTO). Fuel cell research is one of the longest running, if not the longest running, non-defense programs at Los Alamos. Los Alamos continues to serve as a core national laboratory for the DOE Fuel Cell program, as evidenced by two multi-lab projects recently awarded by the Million Mile Fuel Cell Truck (M2FCT) consortium and the ElectroCat consortium, both of which are co-led by Los Alamos. Additionally, Los Alamos is a partner in a third multi-lab project awarded by the H2NEW consortium.

Los Alamos has a breadth of expertise, resources, and technology solutions that support development of hydrogen-related products and applications in the following areas:

### Hydrogen Production

- **Catalysis, separations, and sensing:** Core capabilities include catalyst development, testing, and independent validation; steam methane reforming reactions; and hydrogen purification and separations. Analytical and sensing capabilities include characterization of hydrogen end-use products, online and continuous monitoring of gas phase reactions, and hydrogen leak detection.
- **Electrolysis:** Advanced knowledge, expertise, and capabilities related to low-temperature water electrolysis. Critical components for electrolyzers are under deployment, including PGM-free electro catalysts, polymer electrolyte membranes (including hydrocarbon, alkaline, and high-temperature PEM), porous transport layers, and membrane electrode assemblies (MEAs).
- **Modeling and simulation of production systems and processes:** Design, modeling, and simulation expertise to validate hydrogen production technologies.
- **Biomass and microbial production systems:** Unique capabilities in cultivation and fermentation of microbial systems that can be configured for hydrogen production from waste resources.

Learn more about our hydrogen production capabilities [here](#).

### Hydrogen Storage

- **Underground Storage:** Expertise in long-term underground storage of gases and an extensive knowledge framework for selecting subsurface (geologic) storage sites for both CO<sub>2</sub> and hydrogen. This includes caprock and wellbore integrity assessment, reservoir characterization, transportation infrastructure, and mechanics and leakage monitoring.
- **Geologic storage site selection:** Identification and quantification of biologic and chemical reactions that occur within the different hydrogen subsurface reservoirs being considered. Characterization of diffusive and advective transport properties of hydrogen within these reservoir rocks. Quantification of caprock integrity and sensing strategies for leakage detection. Assessment of technical and economic factors.
- **Materials modeling, validation, and design:** Innovative modeling approaches to investigate fatigue and lifetime characteristics of different hydrogen storage systems, including how defects, fatigue, and damage

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affect safe hydrogen handling operations and inform the selection of optimal materials for hydrogen storage.

Learn more about our hydrogen storage capabilities [here](#).

## Fuel Cell and Hydrogen Conversion

The Los Alamos fuel cell program focuses on polymer electrolyte membrane (PEM) fuel cells, with successions of innovation in:

- High-performance catalysts
- PGM-Free catalysts
- Design and performance of PFSA polymer membranes
- Hydrocarbon Membranes
- Alkaline Membranes
- Gas diffusion layer materials
- Electrodes
- Bipolar Plates
- Flow batteries

Testing facilities at Los Alamos support investigation and validation of the reliability of materials and components as well as overall fuel cell performance and durability.

Los Alamos scientists integrate expertise in theory, modeling, and simulation of electrochemical systems into their overall development efforts. This includes:

- Atomistic scale models to investigate gas and charge transport
- Mesoscale pore network models to understand multi-phase transport
- Capabilities in finite-element methods for multi-scale, fully coupled simulations of system performance

Machine learning approaches are applied to refine electrode catalyst synthesis, as well as fuel cell durability and performance. These capabilities are predominantly utilized for PEM fuel cells but can be readily extended to solid oxide (SOFC), molten carbonate (MCFC), phosphoric acid (PAFC), alkaline (AFC) fuel cells, and other hydrogen related systems. Specifically, Los Alamos has simulation capabilities that can address:

- Understanding the impact of material impurities
- Evaluating defects in fuel cell performance

Learn more about our fuel cell and conversion capabilities [here](#).



## Cross-Cutting Capabilities

**Experimental Resources:** Los Alamos develops and applies analytical methods to evaluate hydrogen reactions, hydrogen detection, materials corrosion, and storage stability. Experimental resources include:

- Hydrogen Safety Sensors
- Hydrogen Quality Sensors
- Low- and high-pressure reactors
- Gas diffusion systems
- Corrosion confinement studies
- Energetic molecular beam sources
- State-of-the-art facilities for materials characterization at multiple scales

**Computation:** As systems engineering is increasingly supported by technical models, our capability in model analysis and calibration brings together models and experimental data.

- Expertise in Bayesian Model Calibration and physics-informed machine learning accelerates system analysis and performance prediction
- Statistical inference methods supports sound reasoning with quantified uncertainty, supporting analysis, and optimization of engineered processes across scales
- Data science for discovery incorporates large data sets in observations and models, particularly relevant to novel materials for efficiency improvements.
- Capability in network science can be used to optimize hydrogen energy systems and infrastructure in the face of complex, interdependent factors.
- High performance computation platforms bring together the co-design awareness of computational platforms, extreme-scale computational models, and best practices in code development.

Learn more about our cross-cutting capabilities [here](#).

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## Brookhaven National Laboratory

Voucher Representative: [Alex Harris](#)

Brookhaven National Laboratory (BNL) works with a range of stakeholders for studies in energy conversion, grid and renewable energy integration, and materials development and integration that are relevant or potentially relevant to hydrogen production and use. BNL also provides access to the DOE designated user facilities NSLS-II and CFN for users to carry out their own material characterization using synchrotron X-ray and nanoscience methods, respectively. BNL has capabilities in the following areas:

### Electrocatalyst research and development

- Fuel cell electrocatalysts: BNL is a leader in fundamentals of electrocatalyst design, synthesis and testing for the hydrogen oxidation reaction (HOR) and oxygen reduction reaction (ORR) in fuel cells.
- Electrolyzer electrocatalysts: Design and testing of electrocatalysts for the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) in electrolyzers.
- Electrocatalyst materials investigated include catalysts with ultralow platinum group metal (PGM) content, including core-shell structures using transition metal alloys, nitrides and related compounds. Investigations also include non-PGM materials including transition metal nitrides, oxynitrides and carbides.
- Capabilities span fundamental materials design, including DFT methods for prediction of catalyst function, to synthesis of nanostructured catalyst materials, electrocatalytic testing, and access to user facilities for in situ studies by synchrotron methods or electron microscopy.

### Hydrogen Production

- Electrolyzer testing
- Electrolyzer integration with PV array

### Energy conversion, including hydrogen blend testing

- Advanced technical solutions in building energy applications, reduced fossil fuel dependence, and technical solutions to reduce combustion related emissions
- Equipped for pilot/bench scale combustion testing of hydrogen blends in various combustion appliances, for instance detailed evaluation for emissions (NO<sub>x</sub>, CO<sub>2</sub> (eq.), CH<sub>4</sub>, or co-pollutants if H<sub>2</sub> blend)
- Strong and existing connection with manufactures to develop burners for “new” fuels
- Ability to accurately analyze the performance of current and emerging heating and power producing equipment with current fossil fuels and hydrogen blends for building energy applications
- Hydrogen blend testing of solid oxide fuel cells (1.5 kW)

### Grid modeling for renewable energy and fuel cell integration

- Steady-state and dynamic models for power grids with renewables including fuel cells
- Development of methods for grid planning, operation, and control

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- Wind energy integration – correlation of wind resource to power generation (expertise to be developed)

## Energy storage integration & optimization

- Size and site optimization for energy storage systems, including thermal storage
- Optimization of Hydrogen bi-directional energy storage system
- Techno-economic analysis to identify optimal configurations for grid, micro-grid and off-grid applications
- Local and integrated measurement methods for H<sub>2</sub> leakage
- Sizing of hybrid energy systems: planning model for hydrogen storage systems
- Integrated wind-hydrogen storage systems for grid services

## Material characterization capabilities

- Discovery and control of materials and chemical processes to revolutionize electrolysis systems
- Elucidation of the structure, evolution, and chemistry of complex interfaces for energy and atomic efficiency
- Multi-modal material characterization expertise for large range of materials including but not limited to membranes, PTLs, electrocatalysts, polymers and metals.
- Develop fundamental understanding of material performance, durability and stability.
- Operando and in situ analysis of materials