Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

HydroGEN: High-Temperature Electrolysis

D. Ding, G. S. Groenewold, H. Ding, M. Li, M. Tucker, R.D. Boardman

Presenter: Dong Ding

Idaho National Laboratory

DOE Hydrogen and Fuel Cells Program

Project WBS 2.7.0.1002 INL HydroGEN 2.0

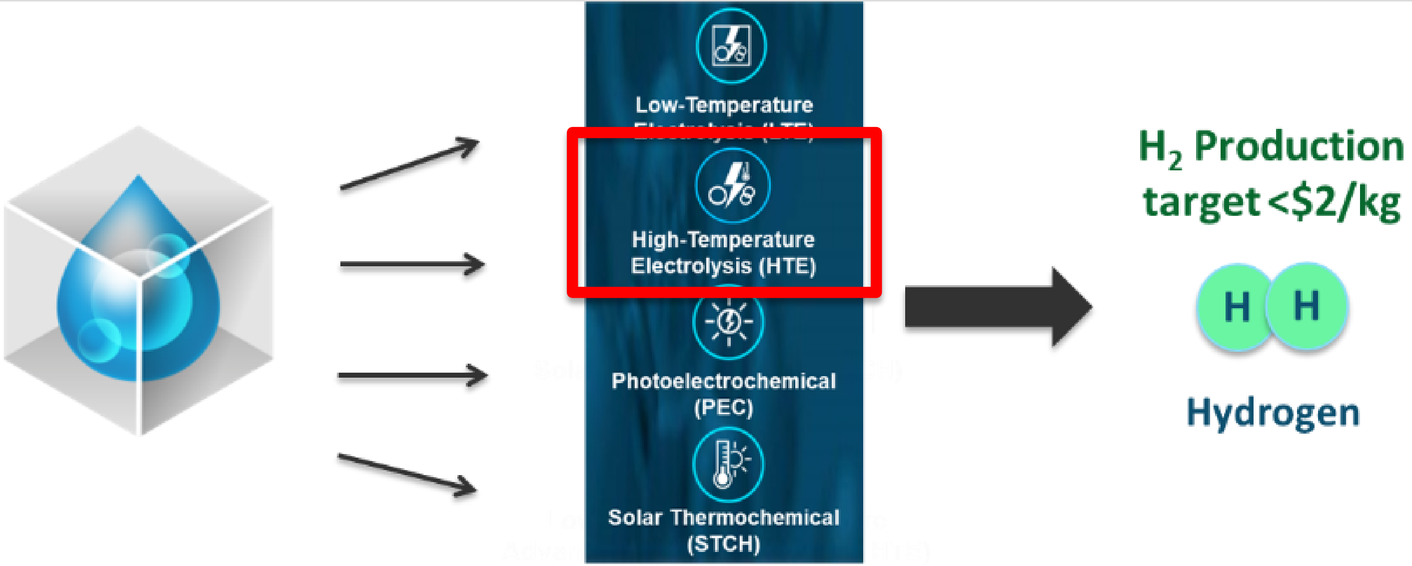
2021 Annual Merit Review

Project ID # P148B

NREL NATIONAL RENEWABLE ENERGY LABORATORY
BERKELEY LAB
Sandia National Laboratories
INL Idaho National Laboratory
Lawrence Livermore National Laboratory
SRNL

HydroGEN: High Temperature Electrolysis Goal

Goal: Accelerate foundational R&D of innovative materials for advance water splitting (AWS) technologies to enable clean, sustainable and low-cost (< $2/kg H_2) hydrogen production.



Low-Temperature Electrolysis (LTE)

High-Temperature Electrolysis (HTE)

Photoelectrochemical (PEC)

Solar Thermochemical (STCH)

H_2 Production target <$2/kg

Hydrogen

HydroGEN is focused on early-stage R&D in H_2 Production

Website: https://www.h2awsm.org/

HydroGEN HTE Overview

Timeline and Budget

HydroGEN 1.0
- Project Start Date: **October 2017**
- FY21 DOE Funding: $240K
- Total DOE Funds Received to Date: $2,627.5K

HTE Supernode
- Project Start Date: **December 2020**
- FY21 DOE Funding (if applicable): $550K
- Total DOE Funds Received to Date: $950K

HydroGEN 2.0
- Project Start Date: **November 2020**
- FY21 DOE Funding (if applicable): $0K
- Total DOE Funds Received to Date: $506.5K

Seedling FOA Projects *HydroGEN Admin budget in this category*
- Project Start Date: **October 2017**
- FY21 DOE Funding (if applicable): **$0K**
- Total DOE Funds Received to Date: **$322.2K**

Seedling project information on individual project slides

Barriers Addressed

- limited cell durability
  - electrolyte|electrode coarsening
  - cation / metal migration
  - pore formation
  - non-conductive phase formation
  - delamination & cracking
  - higher-than-desired production/replacement costs

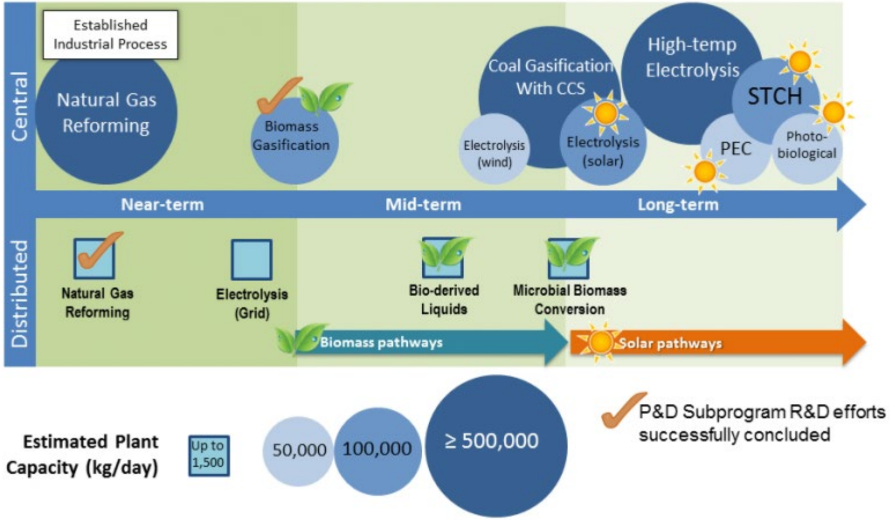
Partners

- PI: Dong Ding, INL
- Co-PIs:
  - Dave Ginley (NREL)
  - Brandon Wood (LLNL)
  - Josh Sugar (SNL)
  - Mike Tucker (LBNL)

- Nexceris
- UTRC
- Saint-Gobain
- Redox
- Univ. Connecticut
- West Virginia Univ
- Univ. South Carolina
- Northwestern University

HTE Relevance/Potential Impact

- HFTO: Expectation that High-Temperature Electrolysis will be a major source of H_2
  - Zero greenhouse gas emissions
  - Clean energy infrastructure
  - Compatible with sources of uninterruptable electricity (nuclear) and renewable electricity
  - Progressing from carbon-emitting technology (natural gas reforming) to zero-carbon emitting technology
  - Potential for next-generation, high paying jobs with excellent diversity and inclusion potential
  - Environmentally benign operations, eliminating environmental justice concerns

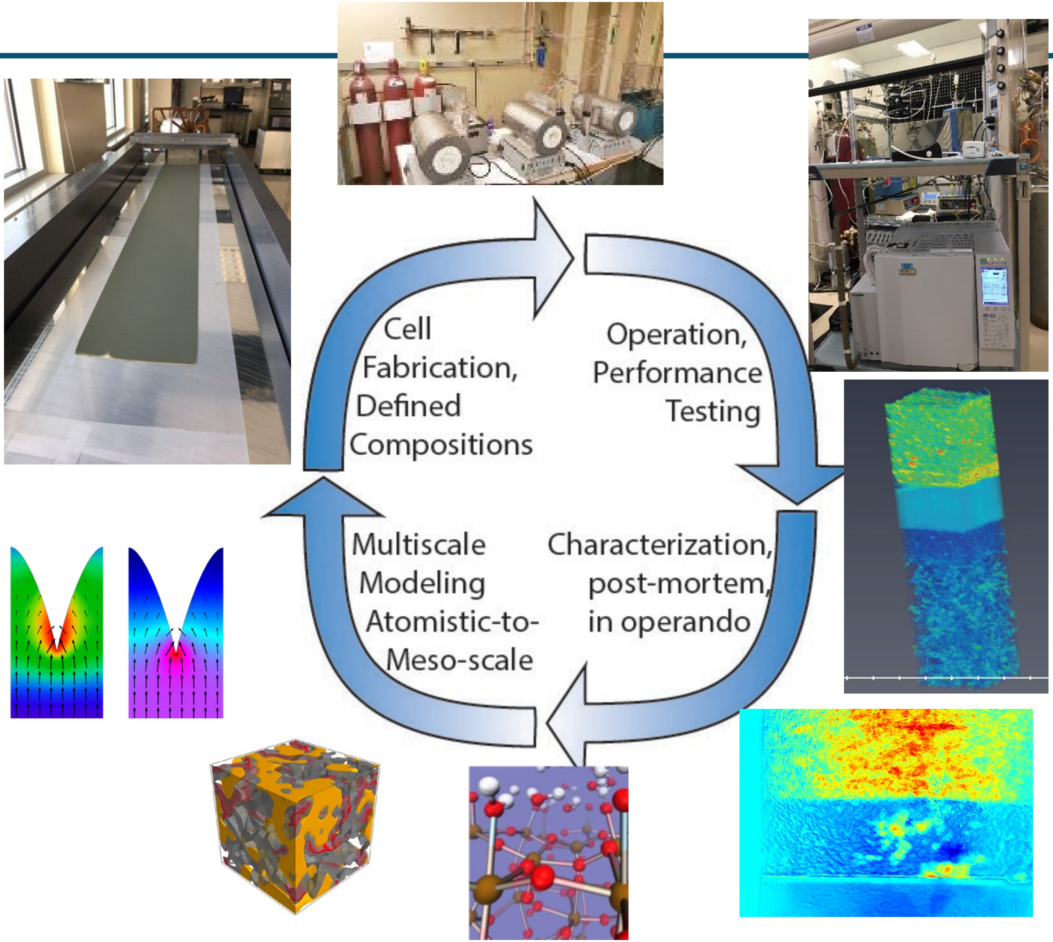


https://www.energy.gov/eere/fuelcells/hydrogen-production-pathways

- Overcoming technology barriers: progress toward improved cell durability leading to competitive economics resulting from lower device costs

HTE Approach

- **Consortium**
  - Interactive, coordinated tasks: fabrication, operation, characterization and modeling
  - Leverage high-powered capability at National Labs
  - Generate a basis for development of new materials and operating strategies
- **Key Milestones**
  - Repeatability of aged button cells - completed
  - Identification of degradation mechanisms - completed
  - Development of initial atomistic models capable of thermodynamic prediction – completed



Cell Fabrication, Defined Compositions

Operation, Performance Testing

Characterization, post-mortem, in operando

Multiscale Modeling Atomistic-to-Meso-scale

Accomplishments / Progress: Nodes for Project Support

Nodes for HTE

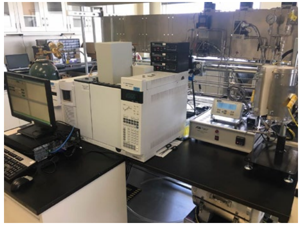
- 9 @ readiness level 1
- 22 @ readiness level 2
- 9 @ readiness level 3

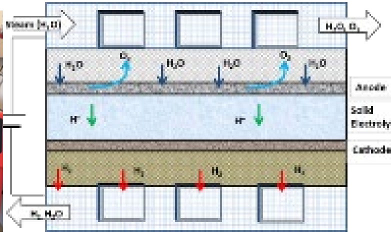
}

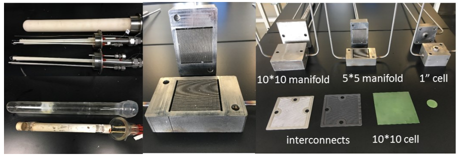
Node Classification

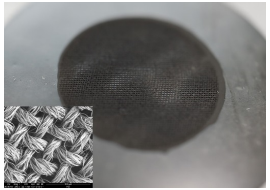
6x Analysis
6x Benchmarking
20x Characterization
13x Computation
6x Material Synthesis
5x Process and Manufacturing Scale-Up
5x System Integration

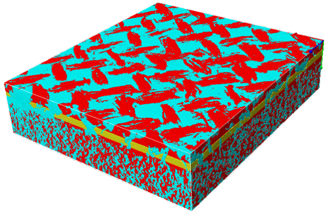
10 nodes used by current HTE projects











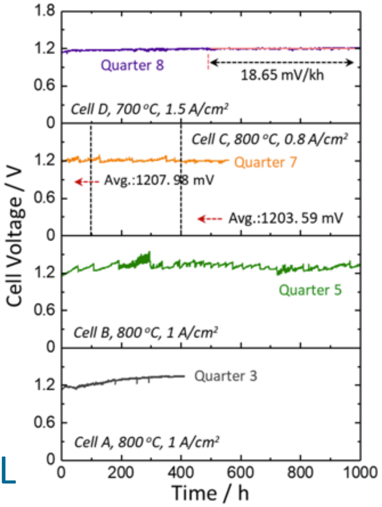
Accomplishments and Progress: **Northwestern University**

PI: Scott Barnett

Northwestern University

Goal and approach

- Goal: Improved o-SOECs that provide stable long-term operation at high current density
- Approach: Degradation mechanisms in oxygen-ion solid oxide electrolysis cells (o-SOECs) are studied using accelerated life testing with varying conditions, materials, and cell designs
- Theory combined with experiment to develop a basic understanding of degradation mechanisms, guide mitigation strategies



Accomplishments in BP2

- High performance solid oxide electrolysis cells developed and shown to operate at high current with low degradation rate of < 20 mV/kh (M5.1, M6.2, BP2 go/no-go target)
- Theory shows effect of Gd-doped Ceria electrolyte layers on oxygen pressure and interfacial fracture (M8.1)
- Initial theory development for predicting Ni migration in Ni-YSZ fuel electrodes (M8.1)
- Substantial reduction in degradation rate of metal-supported electrolysis cells by >100% (M6.1)

Supporting labs: LBNL & INL

Focus of BP3

- Life testing of solid oxide electrolysis cells to determine how operating parameters and cell materials/structures affect different degradation mechanisms (M10.1)
- Completed development of phase-field model of Ni migration in Ni-YSZ under cell operation (M12.1)
- Correlate experiment with theory to develop improved degradation models (M10.1 & M12.1)

Accomplishments and Progress:
Raytheon Technologies Research Center (BP2)

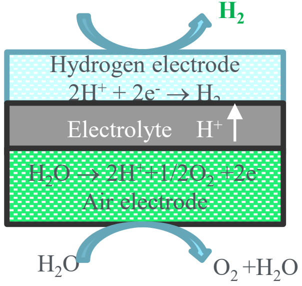
Raytheon Technologies

PI: Tianli Zhu

Concept

Proton conducting electrolyzer

550-650 ℃

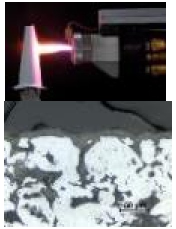


Approach

Integrate low-cost fabrication, material optimization and modeling

Target performance >1.0 A/cm² at 1.4 V and ≤650 ℃

Plasma Spray

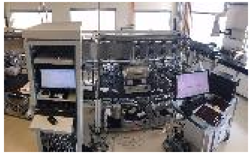


RTRC

Co-sintering

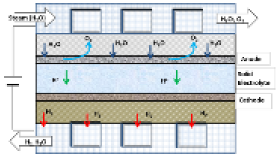
LBNL

Material optimization



INL

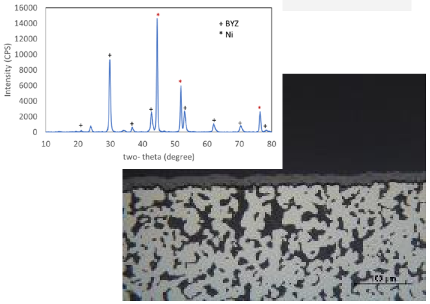
p-SOEC cell modeling



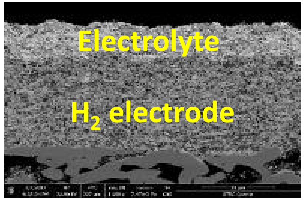
NREL

BP2 Main Accomplishments

Developed suspension plasma spray (SPS) H_2-electrode on porous metal with desired composition and >20%



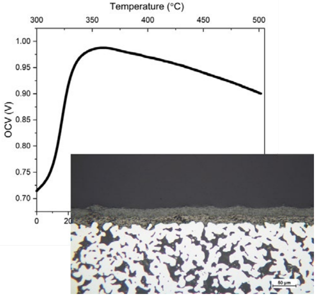
Demonstrated bilayer (H_2 electrode & electrolyte) by plasma spray on porous metal



Remainder BP2 Focus:

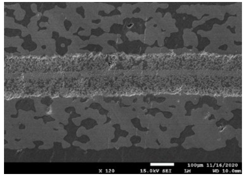
Goal: 0.9 V OCV & >0.8A/cm² at 1.4 V and T≤650 °C

Achieved good OCV, further SPS optimization for better I-V performance



Co-sintering:

- Improve metal sintering to avoid delamination
- Improve OCV



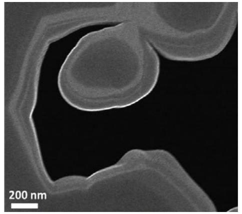
Accomplishments and Progress:
University of South Carolina (BP1)

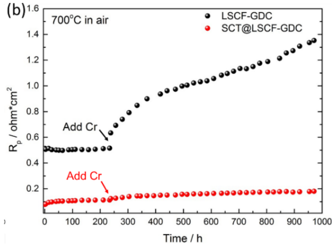
PI: Kevin Huang
Co-PI: Xinfang Jin
Node: INL; NREL

Project Goals: To address oxygen-ion conducting SOEC's degradation problem by developing an isostructural bilayer oxygen evolution reaction (OER) electrode that is electrocatalytically active and Cr-tolerant.

Approaches:

a) Process optimization of isostructural bilayer OER electrode for scale-up fabrication;
b) Manufacturing larger bilayer planar and tubular cells and performance demonstrations at Bench-scale single-planar cell level;
c) Cell performance demonstrations at pilot-scale 2-cell planar stack and single tubular cell level;
d) Understanding performance degradation mechanisms through Multiphysics modeling.



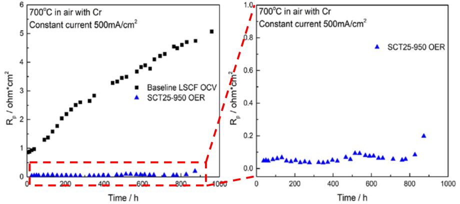


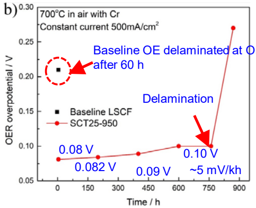
Key technical milestones (BP1):

- Finalize bilayer OE loading and calcination condition
- Finalize OER testing fixture
- Meet button-cell performance: ≤0.15 V OER overpotential at 1 A/cm^2 for 1 kh @ 700 °C
- Establish a Multiphysics model to describe OER degradation mechanisms

Accomplishments in BP1

- Obtained bilayer oxygen electrode (OE) loading, calcination temperature and ASR relationship.
- Demonstrated a new methodology to characterize OER overpotential.
- Achieved bilayer OE OER overpotential <0.15 V at 1 A/cm^2 and 700°C for ~800 hours in Cr-atmosphere.





Focus of BP2

- Study the effect of partial pressure of oxygen on OER polarization ASR.
- Study reversible SOEC/SOFC operation at different current densities.
- Demonstrate long-term stability for 2000 hours in the presence of Cr at 1 A/cm^2 and 700°C.
- Identify failure modes and develop mitigation solutions.

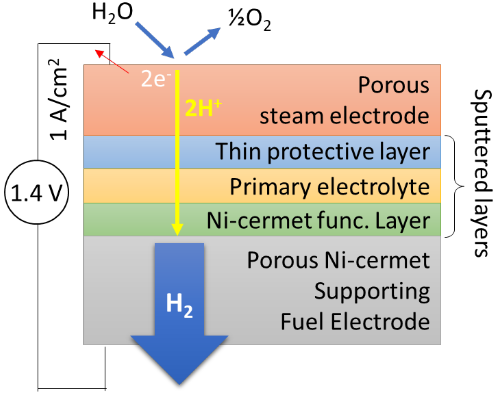
P190, *A Multifunctional Isostructural Bilayer Oxygen Evolution Electrode for Durable Intermediate-Temperature Electrochemical Water Splitting*@1:30 PM Wednesday (6/8)

Accomplishments and Progress:
Redox Power Systems (BP1)

Co-PI: Colin Gore, Bryan Blackburn

Goal and approach

- Redox is using multilayer electrolytes and functional layers to overcome both stability and Faradaic efficiency (FE) challenges in proton conducting SOECs (p-SOEC) by combining materials with different advantages using sputtering, pulsed laser deposition (PLD), and conventional steps
- The approach hinges on using Redox's mature o-SOFC components as substrates for p-SOECs by sputtering and screen printing
- No single electrolyte and electrode offer good stability in high steam (~50%), high Faradaic efficiency (>90%), and acceptable processing temperature (≤1500°C), so Redox is combining materials with different advantages in different layers of the SOEC using scalable sputtering
- Support from **INL** (electrolyte and steam electrode materials) and **NREL** (PLD multilayers) nodes



Metric	State of the Art	Expected Advance
Stability	10-30 mV/kh	< 4 mV/kh
FE	<70% (BZY)	> 95%
Cost	> \$4/kh H_2	< \$2/kg H_2

Accomplishments in BP1

- Stable protective layers deposited by sputtering, tested >200 hours in 50-100% steam at 500°C (no XRD shift or 2nd phase), meeting project milestone M2.1
- Improved Redox o-SOFC support layers for sputtered p-SOECs, testing multilayer cells, reducing defects in later thin film layers
- With INL, made steam electrodes for increased stability in high steam operation compared to $PrBa_{0.5}Sr_{0.5}Co_{1.5}Fe_{0.5}O_{5+\delta}$ (PBSCF)
- With NREL, multilayer electrolytes have been deposited by PLD to evaluate alternative materials. PLD cells are being tested
- Developed automated distribution of relaxation times (DRT) analysis tools for thin film p-SOECs

Focus of BP2

- The goals of BP2 are toward the further improvement of performance parameters, e.g., ASR at 1.4V, FE, OCV
- Deposition parameters will be altered to improve the microstructure and thickness ratio of the electrolytes and functional layer
- Modeling of electronic species (protons, electrons, holes, O^{2-}) will inform the thickness targets for 500 °C operation at high FE
- Improvements in the cell operational stability will continue into BP3 to reach <4 mV/kh at ≥ 1A/cm^2 at 1.4V

P189 Scalable High-Hydrogen Flux, Robust Thin Film Solid Oxide Electrolyzer, @ 2PM, 6/8/21

Accomplishments and Progress:
Nexceris, LLC (BP1)

Project Goal

Develop comprehensive coating strategy to address the critical SOEC degradation mechanisms of metal corrosion and Cr evolution.

Key Impact

Metric	State of the Art	Expected Advance
Degradation Rate	*> 10 mV/kh*	*< 4 mV/kh*
Technology Adoption cost	*> $10/kW*	*< $3/kW*
Current Density *@ 1.4 V/cell*	*> 0.5 A/cm²*	*> 1.0 A/cm²*

Barrier to overcome

Deconvolution of degradation mechanisms- Careful EIS analysis of Cell Performance

Demonstration of coating technology at production relevant scale-use Nexceris' existing stack platform

Approaches

1. Develop high performance o-SOEC cells
2. Develop robust SOEC coating approaches
3. Combine new cell generations with advanced coating approaches
4. Reduce degradation rates
5. Provide advancements at reasonable adoption cost

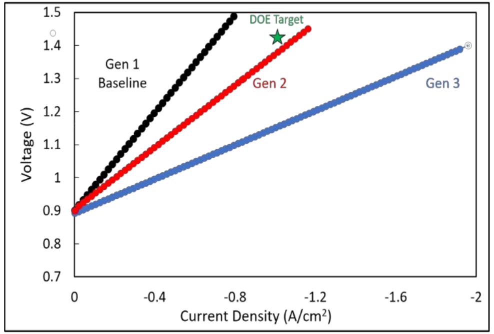
Partner: UCONN

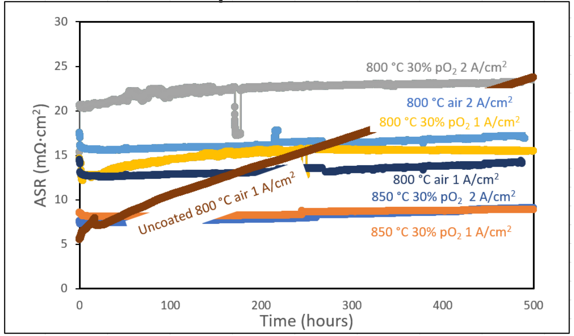
NODES: INL, LBNL

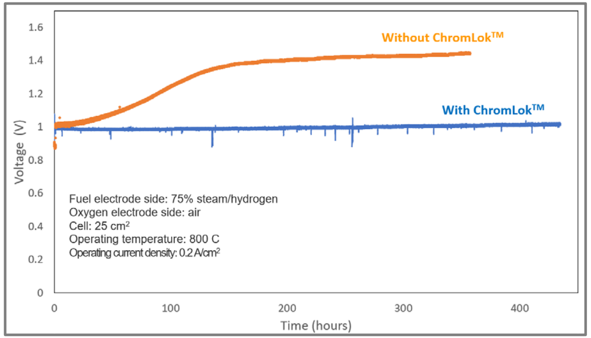
Accomplishments in BP1

1. Demonstrated high performing cells with -2.0 A/cm² @1.4 V
2. Explored advanced IC coatings under aggressive SOEC conditions and current density and demonstrated < 50 mΩ·cm² change for 500 hours
3. Identified up to 5X accelerated IC degradation conditions
4. Demonstrated stable cell operation with ChromLok™ interconnect coating
5. Updated manufacturing cost model with further reduction in cost

Accomplishments in BP1







P188, *Advanced Coatings to Enhance Durability of SOEC Stacks.* Hydrogen Fuel R&D Poster@6:30-8:00 Tuesday (4/30)

Accomplishments and Progress:
West Virginia University (BP2)

PI: Xingbo Liu

Goal: Intermediate-Temperature p-SOECs for simultaneous H_2O splitting and H_2 separation with high current densities > 1.0 A/cm^2 at 1.4 V/cell and durability of <30 mV/1000h while operating at ~600°C (BP2).

Approach:

Electrode and full cell @ WVU

- Modeling driving
  - — H_2O-splitting reaction kinetics
  - — Anode structural and composition
- Candidate anodes development
- Conformal catalyst layer coating
- Cell fabrication and performance measurements

Electrocatalyst @ CSM, NREL, & SNL

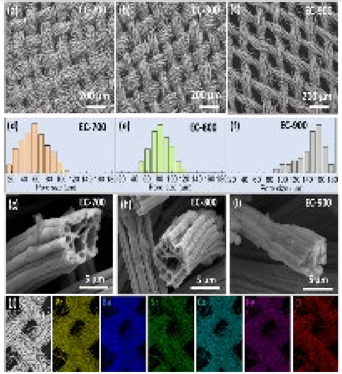
- Appropriate electrocatalyst compositions
  - — High-throughput screening
- Catalysis & local surface activity
  - — Operando ambient-pressure XPS

H-electrolyte & 3D Electrode@ INL:

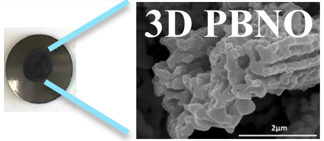
- 3D Textile Electrode
- Conductivity and faradic efficiency improvements

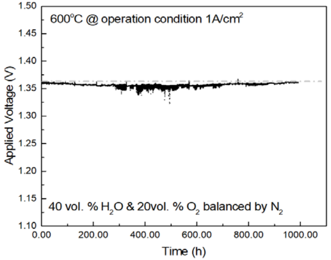
Accomplishment of BP2

- Established and experimentally verified H_2O-splitting reaction kinetics modeling
- E-XPS characterization of O1s and Pr 3d of Pr_2NiO_4 electrode
- Development of highly performing triple conducting anode, ~1A/cm^2 at 1.37V 600°C and durability of <30 mV/1000h
- Ultra-porous electrode skeleton
- Defect chemistry model developed to predict the leakage behaviors of electrolyte under practical conditions
- 3D hierarchical structure anode shows continuous running at current density 1.0 A/cm^2 at <1.4 V at 600°C for 200 h



Morphology, pore size and EDX of the 3D electrode calcined at 700, 800, and 900°C.





p-SOEC cells Running @ 1A/cm^2 600°C

P175, *Intermediate Temperature Proton-Conducting SOEC with Improved Performance & Durability* (Poster)

Accomplishments and Progress: **Saint-Gobain**

PI: Dr. J Pietras, Saint-Gobain
Team: Dr. S Gopalan, Boston Univ.
Dr. O Marina, PNNL
INL, SNL

Project Goal

Develop oxygen electrode materials with high performance in oxygen-ion SOEC which solve the issue of electrode delamination in order to produce hydrogen below the DOE target of $1.87/kg and to test this electrode in a stack platform that has shown degradation rates <0.2%/1000 hours in SOFC mode.

Approach

Novel chemistries of nickelate-based materials with enhanced oxygen hyperstoichiometry will be developed. These materials will be co-sintered in button cells and stacks and tested

Major Technical Milestones

1. Button cell current density >1.5A/cm2 @ 1.3V, <0.75 %/1000 hr post break-in, no electrode delamination observed
2. Short stack current density >1.2 A/cm2, <1%/ 1000 hr

Barriers to be overcome

1) Phase stability/performance: Identification of stable stoichiometry with target electrochemical properties

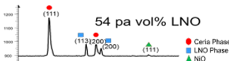
2) Co-sintering with balance of cell: Incorporate materials with stacks ensuring porosity & activity

3) Accelerated testing: Protocol development to probe dominant degradation mechanism

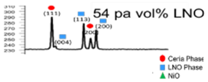
Budget Period 1 Accomplishments

Stabilization

Stabilized LNO in presence of Ceria

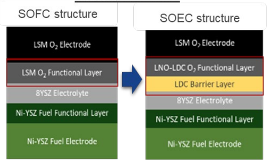


La_2NiO_4 retention

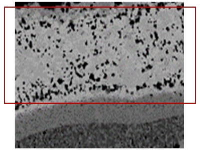


Co-Sintering

Incorporated nickleate within co-sintered cells



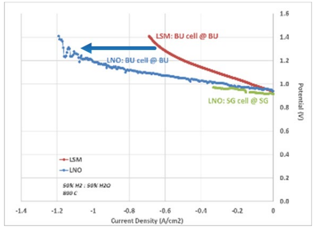
Microstructure achieved



SOEC Performance

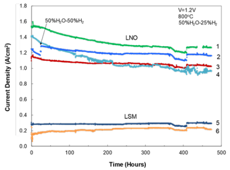
Performance Improvement

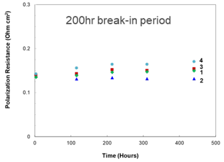
- LNO outperforms LSM electrode
- LNO Cell successfully co-sintered
- Independent of cell design (anode supported and co-sintered cells)



Durability

LNO Showing Stabilization





Budget Period 2 Plan

Utilize the procedures developed and positive results from BP1 to further study:

- Cross family stability fields
- Performance as a function of cation dopants to both barrier layer and the nickelate oxygen electrode
- Extend durability testing to 1000 hours
- Investigate interfacial reaction products
- Down select barrier layer/oxygen electrode pairs for scaling to stack testing

Poster Presentation, p176, non-oral

Accomplishments and Progress: Characterization of Solid Oxide Electrode Microstructure Evolution (HTE Supernode)

Objective: Elucidating HTE failure mechanisms in o-SOEC button cells.

Goals:

- Identify electrode microstructure evolution as a function of local solid-oxide composition and operating conditions
- Correlate with device failure modes
- Rationalize degradation mechanisms
- Develop predictive capability for modeling long term performance
- To develop mitigation approaches for mitigating degradation

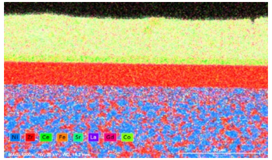
Significance & Impact:

- Comprehensive platform of HTE science and technology available for rapid utilization by HTE developers
- Speed the development of technologies for achieving H_2 production goals

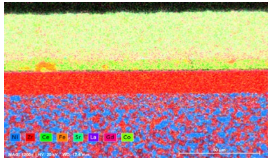
Accomplishments:

- All milestones have been successfully completed
- Dogdibegovic E., Tucker M. et al., J. Power Sources 489 (2020) 229439.

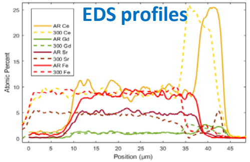
SNL SEM-EDX analysis on SOEC cells after testing

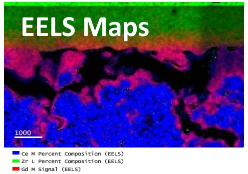


As-received

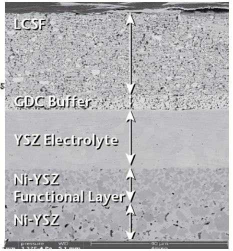


300 hour

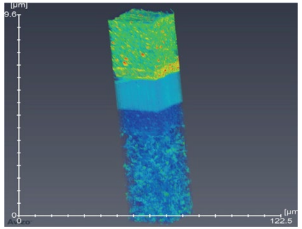




Interlab Button Cell Lifetime Analysis

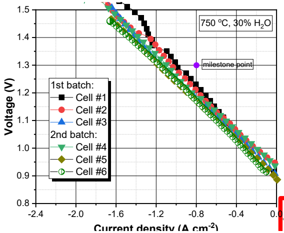


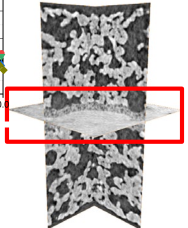
SEM cross-section of **INL** button cell



TEM image of sectioned sample for TXM (**SNL**)

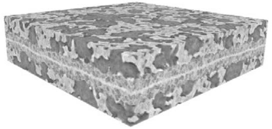
INL synthesized and aged button cells



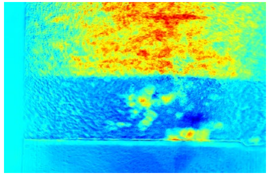


Tomography Imaging (LBNL)

- Resolves cell structure



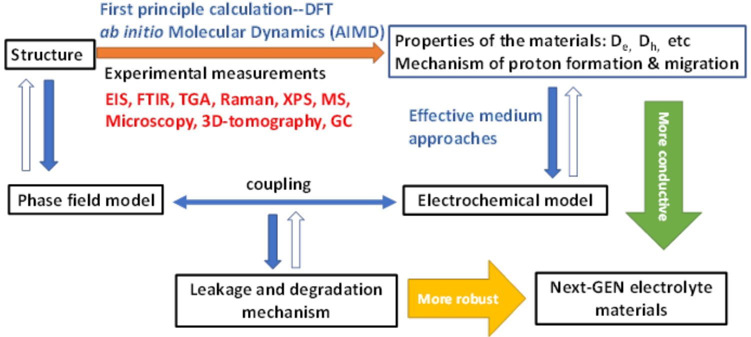
Sectioned sample mounted on TXM beamline at **SLAC**



NREL identified cation migration and void formation

Accomplishments and Progress: HydroGEN 2.0 HTE: proton-conducting solid oxide electrolysis cells (p-SOEC)

Goal: To develop a robust, conductive and reliable electrolyte material system for p-SOEC with high Faradaic efficiency and long durability, by effective combination of advanced computational and experimental effort.



First principle calculation--DFT

ab initio Molecular Dynamics (AIMD)

Structure

Experimental measurements

EIS, FTIR, TGA, Raman, XPS, MS, Microscopy, 3D-tomography, GC

Properties of the materials: D_e, D_h, etc

Mechanism of proton formation & migration

Effective medium approaches

More conductive

Phase field model

coupling

Electrochemical model

Leakage and degradation mechanism

More robust

Next-GEN electrolyte materials

Planned future work:

INL: Study surface environments of electrolyte materials using *in situ* techniques*;* Perform DFT/AIMD calculations to investigate the influences of oxygen vacancies and surface intermediates.

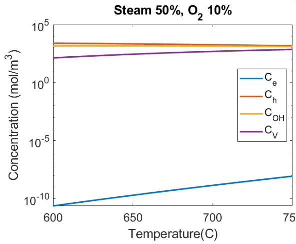
NWU: Calculate charge carrier concentrations under different overpotentials.

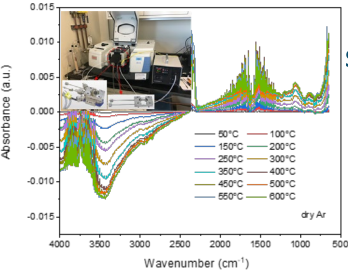
LLNL: Perform large-scale simulation on the influence of working conditions.

Progress

- Demonstrated water adsorption behaviors under operating conditions by *in situ* characterization techniques.
- Evaluated surface properties of DFT/AIMD models and optimized the lattice parameters.
- Studied charge carrier concentrations and their dependence on working temperatures at hydrogen and stream sides by phase-field modeling.
- Investigated the local oxygen partial pressures at the interface of electrolyte/electrode under operation conditions.

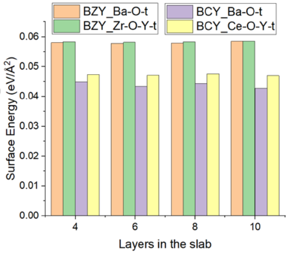
Charge carriers on two sides of electrolyte





***In situ* FTIR spectra of water adsorption vs. temperature on electrolyte material**

Surface energies of models with different layers and terminations



Accomplishments and Progress: Publications and Presentations

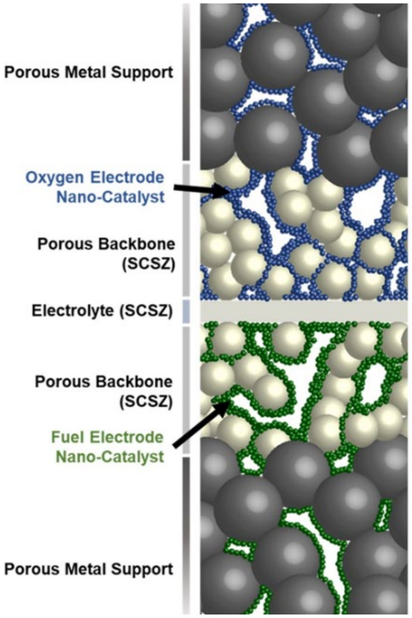
Publications

- Tian, H.; Li, W.; Ma, L.; Yang, T.; Guan, B.; Shi, W.; Kalapos, T. L; Liu X.: Deconvolution of Water-Splitting on the Triple-Conducting Ruddlesden–Popper-Phase Anode for Protonic Ceramic Electrolysis Cells. *ACS Applied Materials & Interfaces 44 (2020) 49574-49585.*
- Ding, H.; Wu, W.; Jin, C.; Hu, B.; Singh, P.; Orme, C.; Ding, D.; et al: Self-sustainable protonic ceramic electrochemical cells using a triple conducting electrode for hydrogen and power production, *Nature Communications 11 (2020) 1907.*
- Tang, W.; Ding, H.; Bian, W.; Wu, W.; Li W.; Liu, X.; Gomez, J.; Vera, Y. R.; Zhou, M.; Ding, D.: Understanding of A-site Deficiency in Layered Perovskites: Promotion of Dual Reaction Kinetics for Water Oxidation and Oxygen Reduction in Protonic Ceramic Electrochemical Cells, *Journal of Materials Chemistry A 8 (2020) 14600-14608.*
- Li, W.; Guan, B.; Yang, T.; Li, Z.; Shi, W.; Tian, H.; Ma, L.; Kalapos, T. L; Liu X.: Layer-Structured Triple-Conducting Electrocatalyst for Water-Splitting in Protonic Ceramic Electrolysis Cells: Conductivities vs. Activity. *J. Power Sources (2021) in press*.
- Wang, Y.; Li, W.; Liu, X.: Degradation of Solid Oxide Electrolysis Cell: Phenomena, Mechanisms, and Emerging Mitigation Strategies – a Review, *Journal of Materials Science & Technology 55 (2020) 35-55*
- Wrubel, J.; Gifford, J.; Ma, Z.; Ding, H.; Ding, D.; Zhu, T.; Modeling the performance and faradaic efficiency of solid oxide electrolysis cells using doped barium zirconate perovskite electrolytes, *Int. J. Hydro. Energy 46 (2021) 11511-11522.*
- Dogdibegovic, E.; Cheng, Y.; Shen, F.; Wang, R.; Hu, B.; Tucker, M.; Scaleup and manufacturability of symmetric-structured metal-supported solid oxide fuel cells, *J. Power Sources 489 (2021) 229439.*
- Jin, X. and Huang, K.; Precautions of Using Three-Electrode Configuration to Measure Electrode Overpotential in Solid Oxide Electrochemical Cells: Insights from Finite Element Modeling, *Journal of the Electrochemical Society*, 167 (2020) 070515.
- Tucker, M.; Progress in metal-supported solid oxide electrolysis cell: A review, *Int. J. Hydro. Energy* 45 (2020) 24203.
- Shen F.; Wang R.; Tucker M.; Long term durability test and post mortem for metal-supported solid oxide electrolysis cells, *J. Power Sources* 474 (2020) 228618.

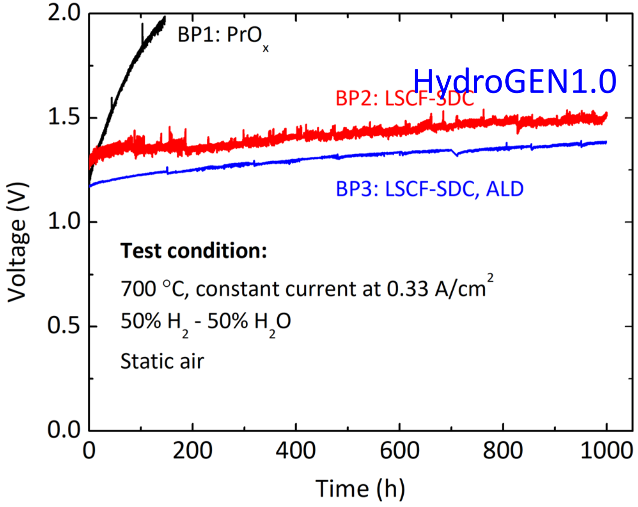
Presentations

- Tian, H.; Li, W.; Liu, X.: Deconvolution of Water-Splitting on Triple-Conducting Anode for Protonic Ceramic Electrolysis Cells. ICACC 2021. Online Virtual meeting. March 24, 2021.
- Tang, W.; Ding, H., Bian, W.; Zhou, W.; Ding, D.: Understanding of A-site Deficiency in Layered Perovskites: Promotion of Dual Reaction Kinetics for Water Oxidation and Oxygen Reduction in Protonic Ceramic Electrochemical Cells. ICACC 2021 Virtual meeting, March 2021.
- Huang, K.: Electrochemical Behavior of Bilayer Oxygen Electrode. ICACC 2021 Virtual meeting, March 2021.

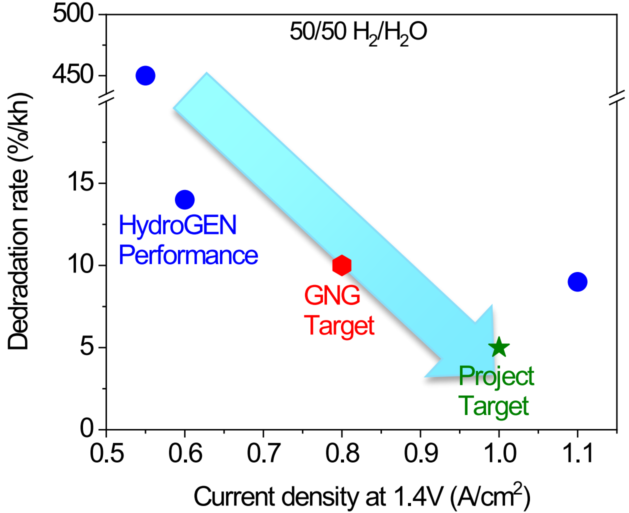
Accomplishments and Progress: HydroGEN 2.0 HTE: Metal-supported solid oxide electrolysis cells (MS-SOEC)



Button Cell Progress



Test condition:
700 °C, constant current at 0.33 A/cm^2
50% H_2 - 50% H_2O
Static air



Improvements:

- Oxygen electrocatalyst composition
- ALD coating on metal support to suppress Cr migration

Future Work:

- Constant-V vs. Constant-I behavior
- Improve oxygen catalyst
- Thicker, more scalable coating
- Leverage cell structure improvements from MS-SOFC

Future Work

Future Work:

- Constant-V vs. Constant-I behavior
- Improve oxygen catalyst
- Thicker, more scalable coating
- Leverage cell structure improvements from MS-SOFC

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

HTE Collaboration & Coodination

Project-driven tech transfer, resulting in

- **Efficiency**
- **Yield**
- **Cost**
- **Durability**
- **Manufacturability**

HTE Node Labs

INL Idaho National Laboratory

NREL National Renewable Energy Laboratory

Sandia National Laboratories

Berkeley Lab

Lawrence Livermore National Laboratory

Supernode

Support through:

Personnel

Equipment

Expertise

Capability

Materials

Data

Interactive HTE Projects

p-SOEC

Raytheon Technologies

University of Connecticut

West Virginia University

REDOX Redox Power Systems, LLC

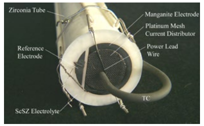
o-SOEC

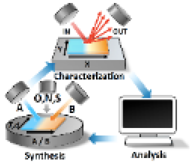
Northwestern University

Saint-Gobain

University of South Carolina

Nexceris where energy meets environment





HTE Remaining Challenges and Barriers

- Mitigating electronic leakage while maintaining cell performance, and materials durability in the p-SOEC devices and materials
- Accurate modeling across multiple scales with improved accuracy to rationalize, predict and control

HydroGEN 2.0 - HTE Proposed Future Work

- Definitive understanding surface environments of electrolyte materials using in situ techniques
- Maturation of DFT/AIMD calculations describing the effects of oxygen vacancies and surface intermediates
- Complete charge carrier concentrations as a f(overpotential) (NWU)
- Develop large-scale simulation that accurately describes effects of salient operating parameters (LLNL)

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

HTE Summary

- p-SOECs
  - lower operating temperatures, promising improved materials and device durability and lifetimes
  - equal or improved conversion performance
  - water adsorption phenomena defined during operation using in situ characterization
  - DFT/AIMD approaches optimized, evaluated for surface modeling
  - Significant improvement in understanding effects of temperature on charge carrier concentrations at both the steam and hydrogen electrode interfaces, using phase-field modeling
  - Significant improvement in the understanding of oxygen partial pressures of electrolyte/electrode interface at typical operation conditions.
- MS-SOECs
  - Significantly improved oxygen catalyst composition, improved metal coatings to mitigate Cr migration
- o-SOECs
  - Detailed understanding of degradation mechanisms, development of in operando characterization tools, and multiscale modeling, setting stage for transition to H2NEW

Technical Backup and Additional Information

Technology Transfer Activities

- Tech transfer in the HydroGEN HTE project occurs organically via partner programs with commercial collaborators
  - Raytheon Technologies: development of new p-SOEC technology
  - Redox: sputtering and pulsed laser desorption fabrication applications, PBSCF electrodes
  - Saint Gobain: exceptional resistance to degradation at high current densities in new o-SOECs
  - Nexceris: high performing cells operating at high current densities, advanced interconnect coatings functioning under aggressive SOEC conditions
- Patent Applications
  - D. Ding, H Ding, W. Wu and C. Jiang. Reversible Solid oxide Cell Operated with A High-Performing and Durable Anode Material for hydrogen and power generation at intermediate temperatures. US Patent Application (16/560, 719), 2019.
  - D. Ding, H. Ding, W. Wu and C. Jiang. Electrochemical cells for hydrogen gas production and electricity generation, and related structures, apparatuses, systems, and methods. US Patent Application (17/309, 012), 2021.
  - T. He, D. Ding, W. Wu. Methods and systems for hydrogen gas production through water electrolysis, and related electrolysis cells. US Patent Application (16/483,631), 2019.

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West Virginia University
Northwestern University
NEXCERIS where energy meets environment
REDOX
Redox Power Systems, LLC
UNIVERSITY OF SOUTH CAROLINA

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

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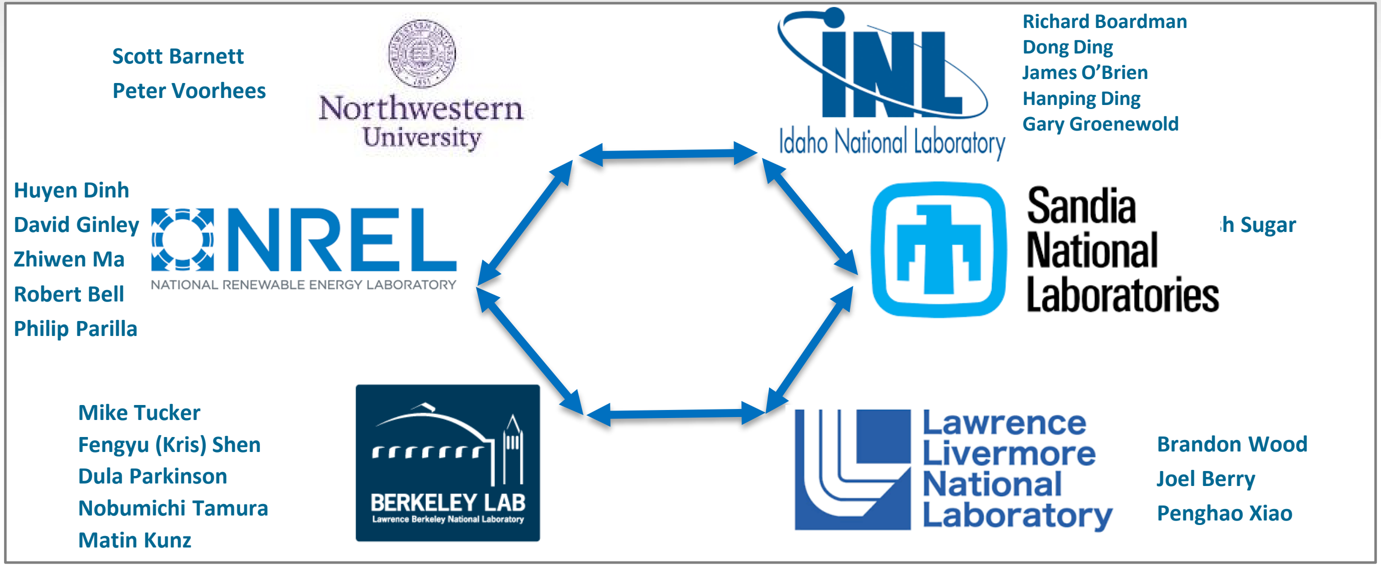
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

HTE Supernode Team - 18 experts



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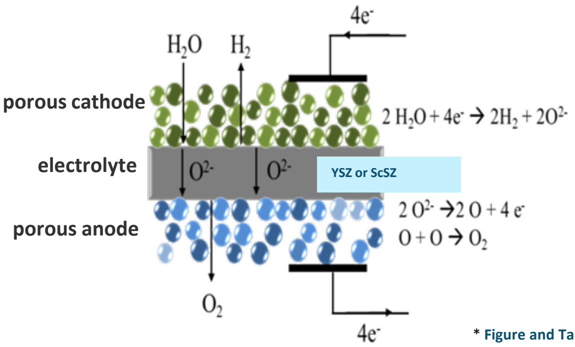
Lawrence Livermore National Laboratory
SRNL

Overview – HTE Technology, o-SOEC, p-SOEC

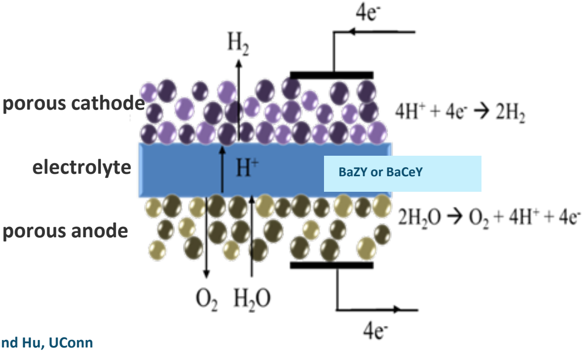
Oxygen Ion Transport Solid-Oxide Electrolysis*

(O^{2-} -SOEC; Unresolved R&D Material Barriers Remain)



Proton-Conducting Solid-Oxide Electrolysis*

(H^+-SOEC; Early-Stage Research Needed)

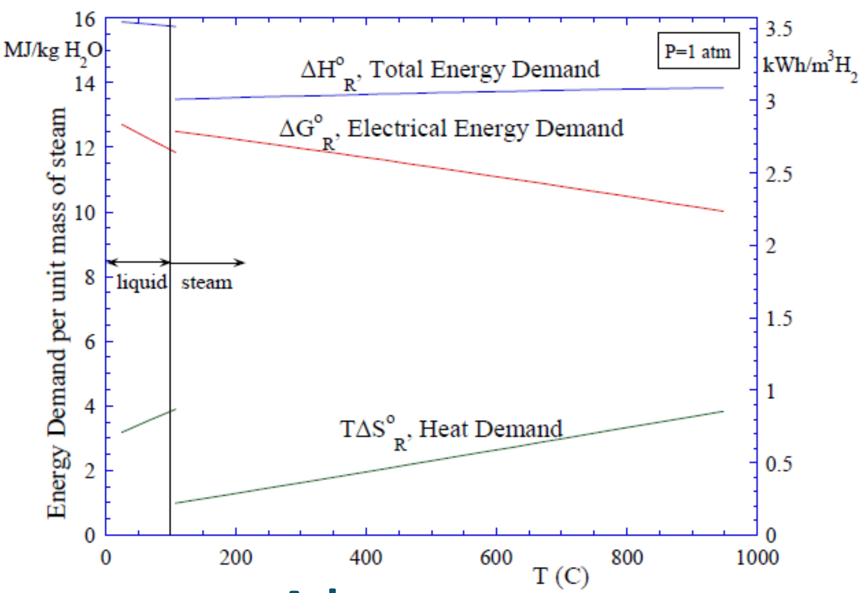


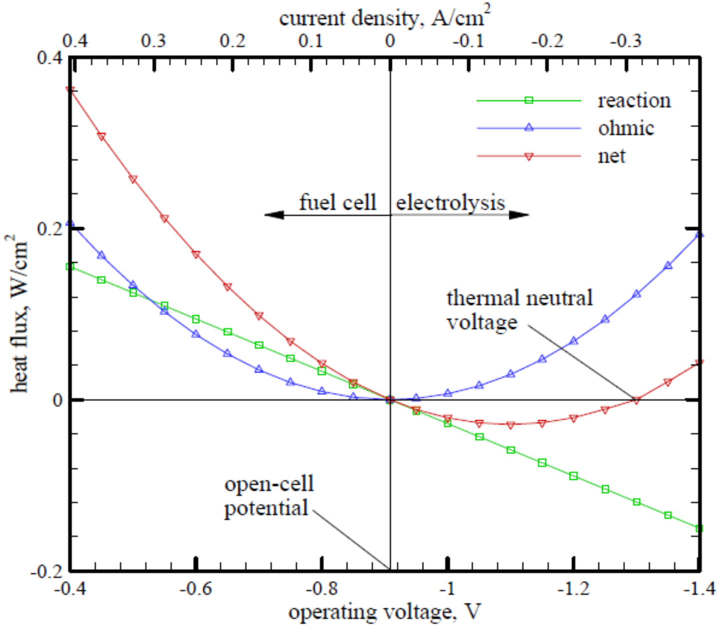
* Figure and Table Adapted from: Singh and Hu, UConn

O^{2-}- SOEC	Attributes	H^+- SOEC
650-850°C	Operating Temperature	550-750°C
0.015 $S.cm^{-1}$ at 850°C	Electrolyte Conductivity	0.01 $S.cm^{-1}$ at 650°C
$H_2O + H_2$	Cathode Products	Pure H_2
$H_2O + O_2$	Anode Products	O_2 + sweep gas
durability decreases: microstructure evolution, D stresses, Cr migration	Challenges	slower kinetics, maturation of electrolyte (synthesis, densification, H^+ conduction)

HTE Supernode & H2NEW is focused on attacking o-SOEC issues: elemental migration, unexpected phase formation, crack and void formation, and delamination

Overview: Advantages/Challenges of HTE





Advantages

- 30-50% higher thermodynamic efficiency possible for steam v. water splitting (free energy + electricity use)
- Reversible operation possible with optimal design of cells, stacks and modules
- Does not require precious metals

Challenges

- cell degradation, *viz.*, sintering, pore consolidation, Cr migration / poisoning, catalyst deactivation (Ni hydridation), delamination