H2NEW: Hydrogen (H2) from Next-generation Electrolyzers of Water Overview

Director: Bryan Pivovar, National Renewable Energy Laboratory (NREL)

Deputy Director: Richard Boardman, Idaho National Laboratory (INL)

Date: 6/6/2023

DOE Hydrogen Program
2023 Annual Merit Review and Peer Evaluation Meeting

Project ID # P196

Project Goals

Goal: H2NEW will address components, materials integration, and manufacturing R&D to enable manufacturable electrolyzers that meet required cost, durability, and performance targets, simultaneously, in order to enable $2/kg hydrogen (by 2026 on way to H2 Shot target, $1/kg by 2031).
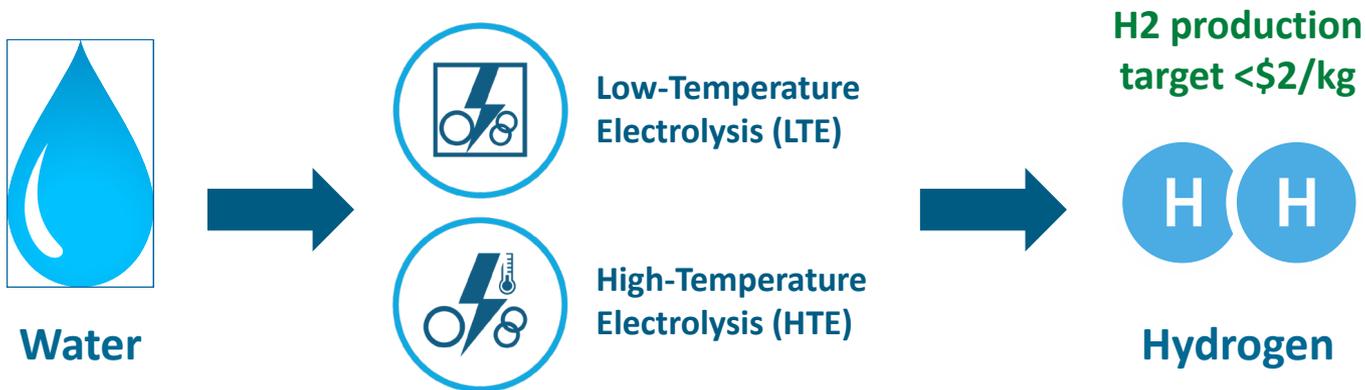
H2NEW has a clear target of establishing and utilizing experimental, analytical, and modeling tools needed to provide the scientific understanding of electrolysis cell performance, cost, and durability tradeoffs of electrolysis systems under predicted future operating modes

Overview

Timeline and Budget

- Start date: **October 1, 2020**
- FY21 DOE funding: **$10M (75% PEM, 25% O-SOEC)**
- FY22 DOE funding: **$10M (75% PEM, 25% O-SOEC)**
- FY23 DOE funding: **$28M (45% PEM, 20% LA, 35% O-SOEC)**

Detailed AMR posters on each task:

- **https://www.hydrogen.energy.gov/amr-presentation-database.html** (search H2NEW)

Consortium Team*

- NIST, SLAC
- UC-Irvine
- Carnegie Mellon Univ
- Colorado School of Mines

* Expansion to include additional academic and industrial partners through FOA projects currently under review

Potential Impact – H2NEW connection to H2@Scale

Illustrative example, not comprehensive
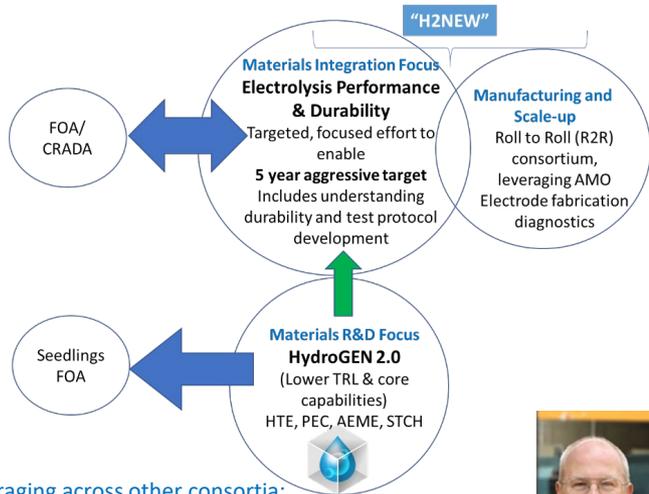https://www.energy.gov/eere/fuelcells/h2-scale
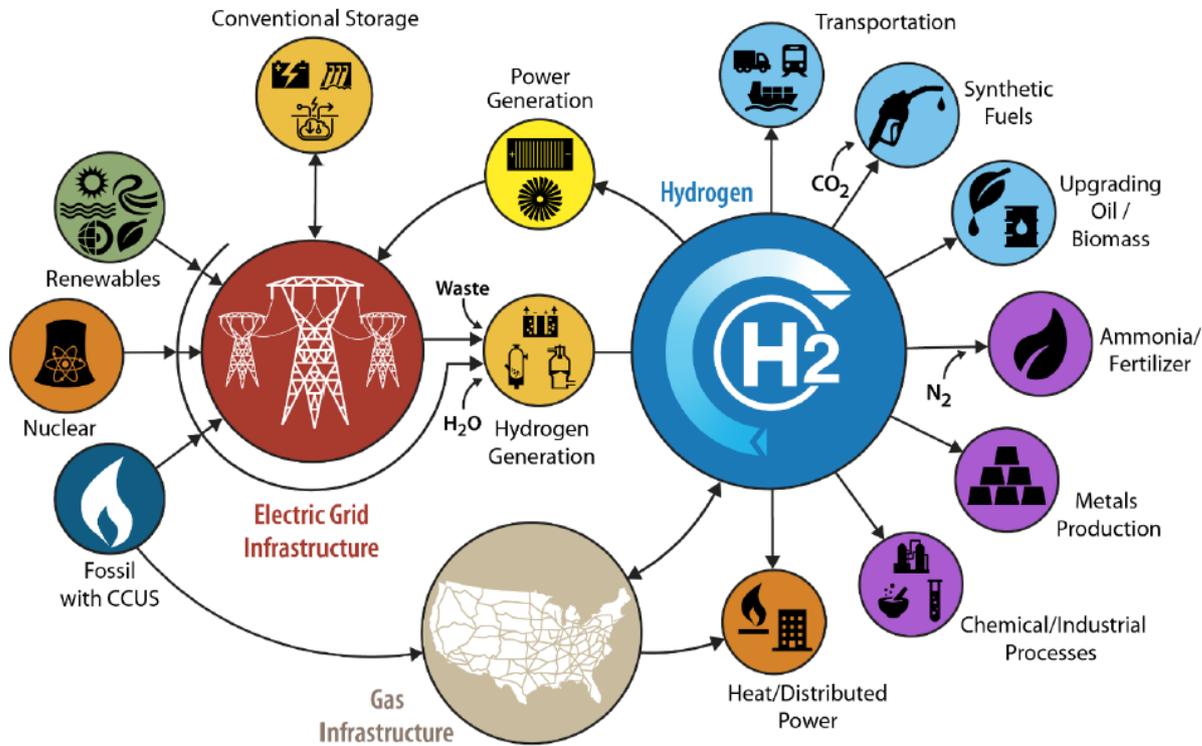
- Making, storing, moving and using H2 more efficiently are the main H2@Scale pillars and all are needed.

- Making H2 is the inherently obvious, first step to spur the wide-ranging benefits of the H2@Scale vision.

- Electrolysis has most competitive economics and balances increasing renewable generation challenges.

Consortium Structure
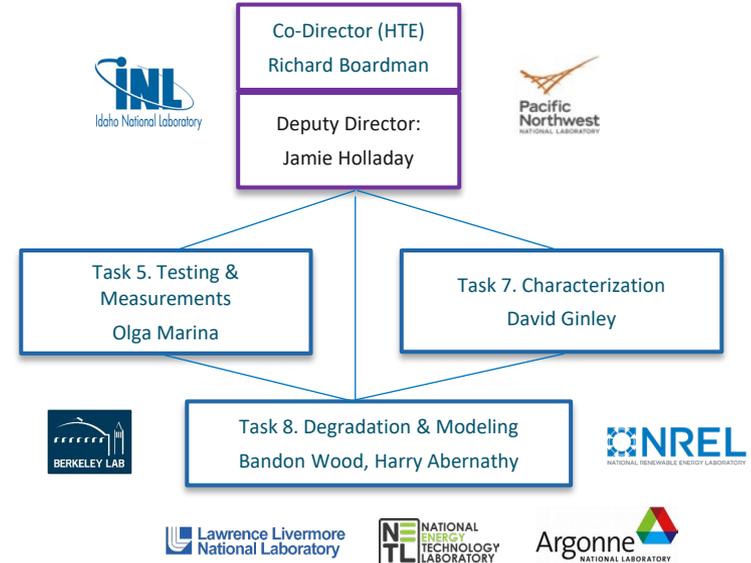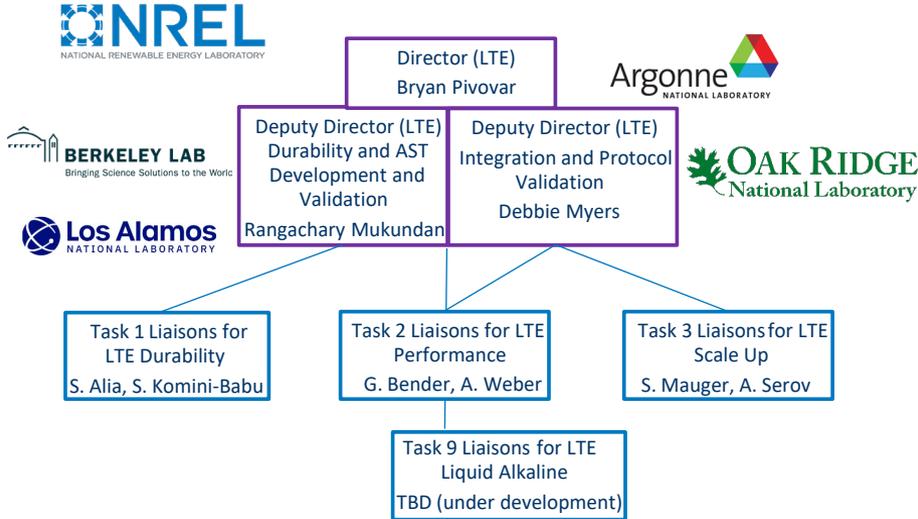
- Well developed cross-lab structures for PEM and O-SOEC
- Liquid Alkaline efforts under development but will feed into LTE management structure

Collaborations and Coordination

PEM Stakeholder Advisory Board Members

Kathy Ayers VP R&D Nel Hydrogen

Cortney Mittelsteadt VP Electrolyzer Technology Plug Power

Andy Steinbach Specialist Materials Science 3M

Jack Brouwer Professor U.C. Irvine

Mark Mathias Consultant retired (GM)

Liquid Alkaline Stakeholder Advisory Board (under development)

Associate Lab Director Board (in place)

HTE Stakeholder Advisory Board Members

Scott Swartz Founder & CTO Nexceris

Xiao-Dong Zhou Prof. Chem. Eng. Univ. of Louisiana-Lafeyette

Greg Tao Vice President Chemtronergy

Bryan Blackburn Chief Tech. Officer Redox Power Systems

John Piatras Sr. Principal Scientist, Group Leader Saint-Gobain
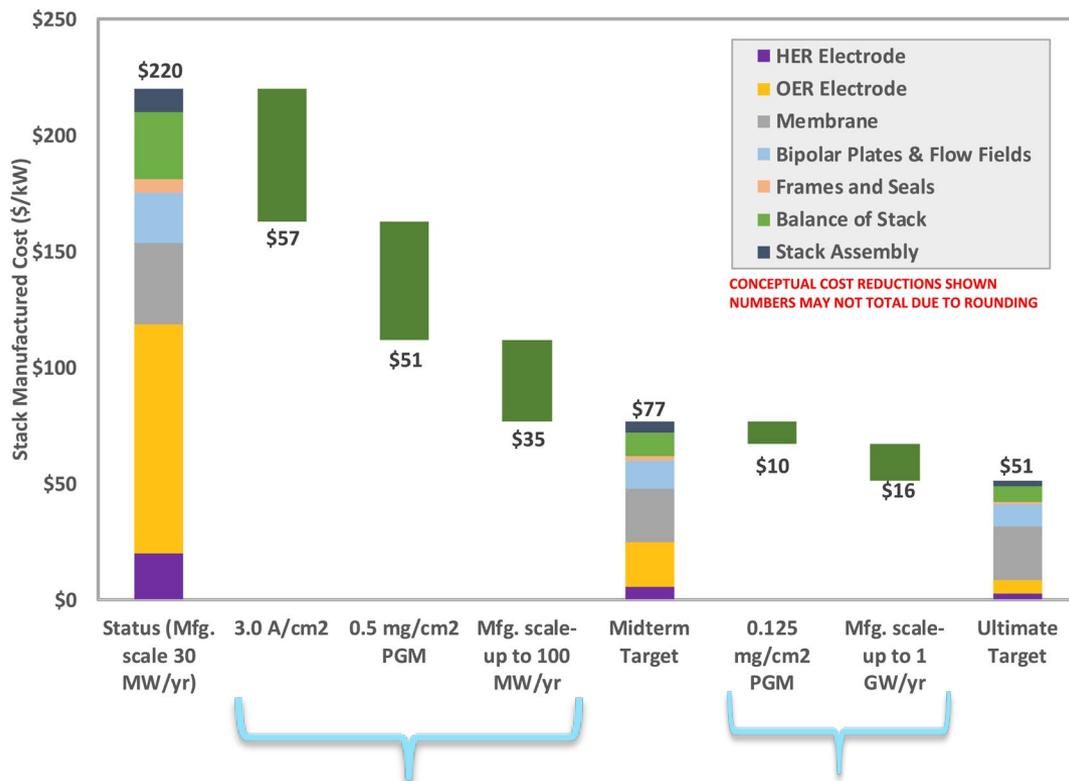
Elango Elangovan VP of Research OxEon Energy

Joe Hartvigsen Co-Founder & CEO OxEon Energy

Tony Leo Chief Tech. Officer & Exec. VP FuelCell Energy

Scott Barnett Prof. Materials Sci. & Engineering Northwestern University

- Leveraging across other consortia:
- HydroGEN 2.0 (HFTO)
- ElectroCat 2.0 (HFTO)
- Million Mile Fuel Cell Truck (HFTO)
- Roll to Roll (Under development)
- Numerous industrial, academia, and international interactions: (IEA, ASTWG, materials suppliers, informal collaborations)
- Select group of advisors representing OEMs, Tier 1 suppliers, analysis and manufacturing interests.

H2IQ Webinar: https://www.energy.gov/eere/fuelcells/january-h2iq-hour-h2new-consortium-overview-electrolyzer-development-capabilities-0

Potential Impact: Stack Costs (PEM)

Waterfall chart — Stack Manufactured Cost ($/kW):

- Status (Mfg. scale 30 MW/yr): $220
- 3.0 A/cm2: $57
- 0.5 mg/cm2 PGM: $51
- Mfg. scale-up to 100 MW/yr: $35
- Midterm Target: $77
- 0.125 mg/cm2 PGM: $10
- Mfg. scale-up to 1 GW/yr: $16
- Ultimate Target: $51

Legend:
- HER Electrode
- OER Electrode
- Membrane
- Bipolar Plates & Flow Fields
- Frames and Seals
- Balance of Stack
- Stack Assembly

CONCEPTUAL COST REDUCTIONS SHOWN
NUMBERS MAY NOT TOTAL DUE TO ROUNDING

| Stack Targets	Status	2026	Ultimate
Cell (A/cm^2)	2.0	3.0	3.0
Cell voltage (V)	1.9	1.8	1.6
Lifetime (khr)	40	80	80
Degradation (mV/khr)	4.8	2.3	2.0
Capital Cost ($/kW)	450	100	50
PGM loading (mg/cm^2)	3	0.5	0.125

https://www.energy.gov/eere/fuelcells/technical-targets-proton-exchange-membrane-electrolysis

These 3 areas

1. Increased efficiency/current density
2. Decreased PGM loading
3. Scale-up

Are the strongest levers for addressing stack costs and primary focus of H2NEW.

Potential Impact: Hydrogen Levelized Cost
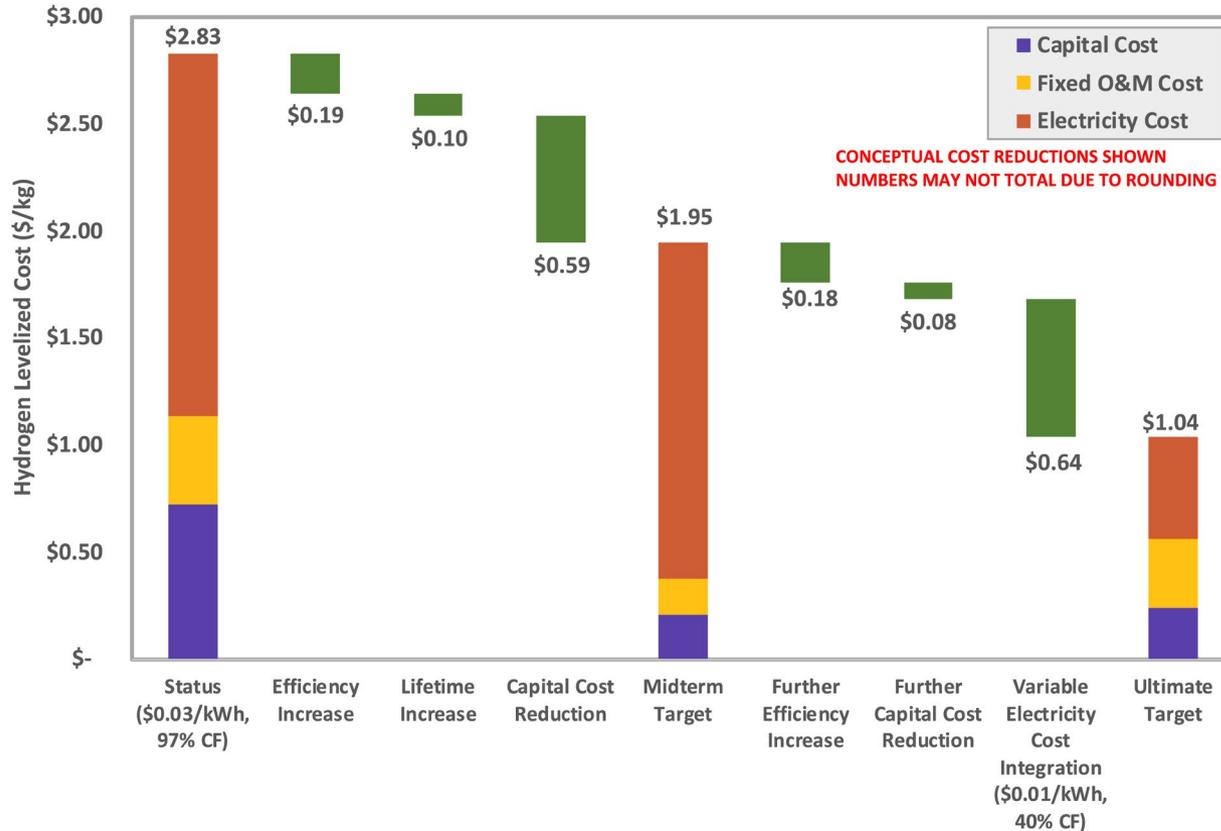
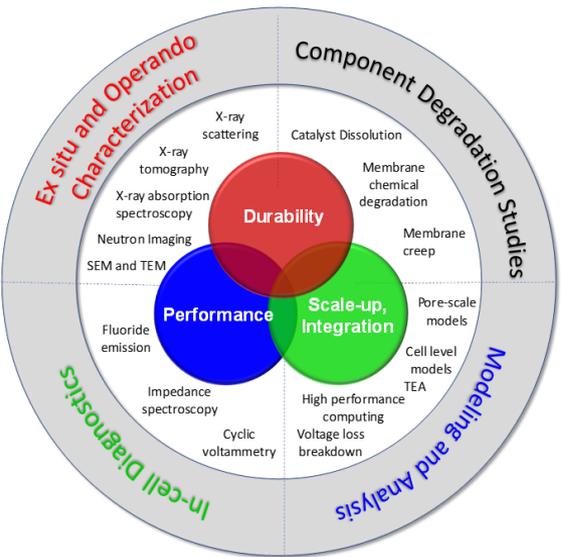

Select pathway to $2/kg and $1/kg identified.

Much of HLC gains possible through greatly decreasing capital costs and enabling lower cost electricity through variable operation.

These advances can't come with compromised durability or efficiency, so all three areas are linked.

Approach: H2NEW Cross-technology Methodology

- Durability
  - Establish fundamental degradation mechanisms
  - Develop accelerated stress tests
  - Determine cost, performance, durability tradeoffs
  - Develop mitigation
- Performance
  - Benchmark performance
  - Novel diagnostic development and application
  - Cell level models and loss characterization
- Scale-up
  - Transition to mass manufacturing
  - Correlate processing with performance and durability
  - Guide efforts with systems and technoeconomic analysis

H2NEW Poster Presentations*
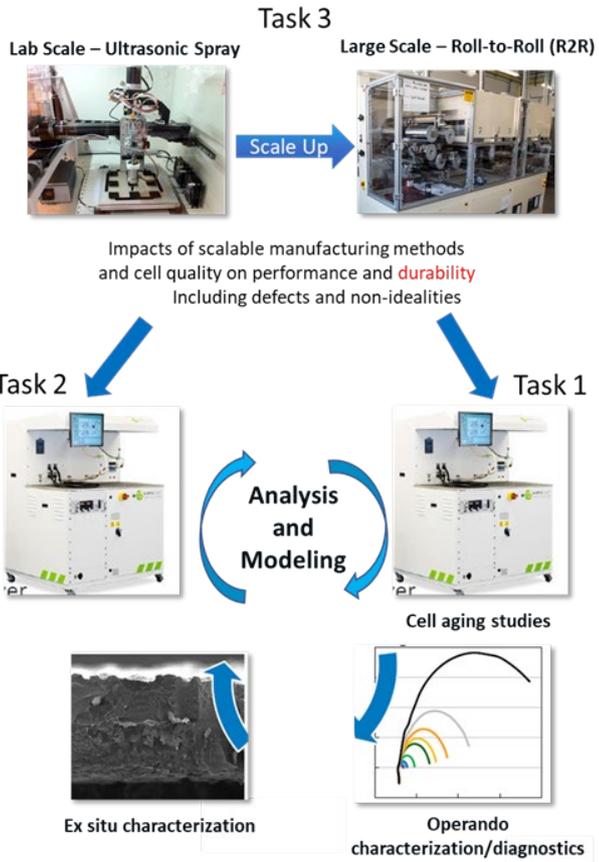
- **Polymer Electrolyte Membrane (PEM)**
  - Task 1: Durability and AST Development:
    https://www.hydrogen.energy.gov/pdfs/review23/p196a_mukundan_2023_p.pdf
  - Task 2: Benchmarking and Performance:
    https://www.hydrogen.energy.gov/pdfs/review23/p196b_myers_2023_p.pdf
  - Task 3: Manufacturing, Scale-Up, and Integration:
    https://www.hydrogen.energy.gov/pdfs/review23/p196c_mauger_2023_p.pdf
  - Task 3c: System and Technoeconomic Analysis:
    https://www.hydrogen.energy.gov/pdfs/review23/p196d_badgett_2023_p.pdf

- **Liquid Alkaline (LAWE)**
  - Task 9: Liquid Alkaline: https://www.hydrogen.energy.gov/pdfs/review23/p196h_shviro_2023_p.pdf

- **Oxide-conducting – Solid Oxide Electrolysis (O-SOEC)**
  - Task 5: Durability and AST Development:
    https://www.hydrogen.energy.gov/pdfs/review23/p196e_marina_2023_p.pdf
  - Task 7: Cell Characterization: https://www.hydrogen.energy.gov/pdfs/review23/p196f_ginley_2023_p.pdf
  - Task 8: Multi-Scale Degradation Modeling:
    https://www.hydrogen.energy.gov/pdfs/review23/p196g_wood_2023_p.pdf

*Additional details found in associated <u>2023 AMR posters</u> websites provided

H2NEW Activities: Low Temperature Electrolysis (LTE)

Approach: Select LTE Milestones*

Milestone Name/Description	Due Date	Type	Status
Updated version of DFMA cost analysis report for HFTO and external stakeholder review (NREL)	12/31/2022	QPM	Complete
Define LAWE system configuration and identify all components of subsystems for gas and liquid control, hydrogen purification and electrical power supply. (ANL, NREL)	12/31/2022	QPM	Complete
Establish the correlation of the in-situ performance (polarization curve, EIS, CV) to the changes in morphology on the different break-in procedures. (LANL/ANL/ORNL/NREL)	3/31/2023	QPM	Complete
Model the stability of catalysts and separators based on ex situ and operando experimental data and support the development of accelerated stress tests (ASTs) (NREL, LANL, ORNL, ANL, LBNL)	6/30/2023	QPM	On Track
Complete durability testing under steady state operation and dynamic operation over 3 voltage windows. Validate the IrO2 dissolution model by comparing OER kinetic over potential increase observed in cell-level AST experiments to those predicted from dissolution-based models. Propose and validate at least one mitigation strategy to improve the durability of electrolysis cells under dynamic operation (NREL, LANL, ANL, LBNL)	9/30/2023	Mile-stone	On Track
Demonstrate LAWE single-cell performance agreement evaluated at 0.6 A/cm2, at less than or equal to 1.8V, and within +/- 50mV for at least three H2New labs at an operating temperature greater than or equal to 60C.	9/30/2023	Mile-stone	On Track
In coordination with HFTO, establish methodology involving analytical assumptions of electricity price, operating cycle, stack cost, performance and durability for evaluating hydrogen levelized costs and progress towards meeting the H2NEW target of $2/kg by 2026 and the Hydrogen Shot target of $1/kg by 2031. (all labs)	9/30/2023	Mile-stone	On Track

*Partial list, see associated 2023 AMR posters for additional details

Accomplishments

- 2023 AMR Select Highlights
  - Task 3c – Systems/Technoeconomic Analysis
    - Future electricity markets
    - Turndown ratio impact
  - Task 1 - Durability
    - Ir dissolution – Potential cycling
    - Establishing degradation baselines
    - Start/Stop – Reference Electrodes
    - AST Development
  - Task 2 - Performance
    - Benchmarking
    - Pressure effects
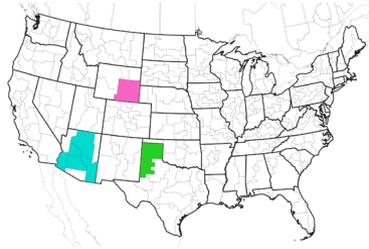   - Test capability development
    - Cell modeling
  - Task 3 – Scale-up
    - Catalyst ink stability
    - R2R catalyst layer durability
  - PTL (cross task effort)
    - Novel tunable PTL/MPL development
    - PTL/CL interface optimization
    - Operando characterization of PTLs
  - Task 9 – Liquid Alkaline
    - Reference system
    - Benchmarking
    - Cell modeling
    - Initial performance testing

https://www.hydrogen.energy.gov/pdfs/review22/p196_pivovar_boardman_2022_o.pdf

Low Temperature Electrolysis (LTE)

Task 3c: Analysis (more content in AMR Poster <u>P196d</u>)

Accomplishment: Analysis of projected marginal electricity costs by location

Palo Verde, AZ

2022 NREL cambium data
Mid-case with
100% decarb by 2035
Zone p28, Palo Verde, AZ

Amarillo, TX
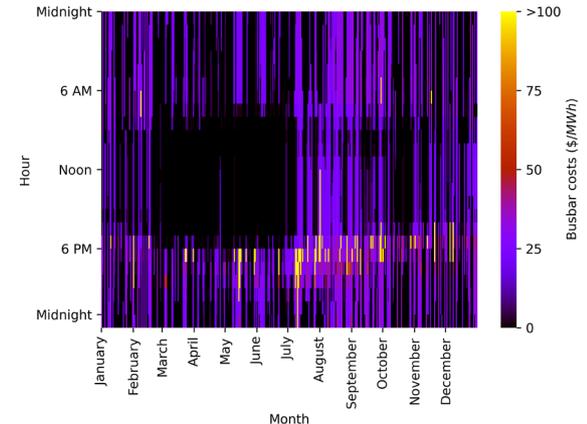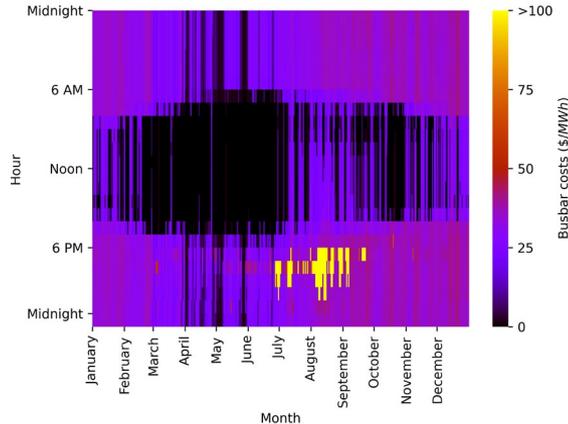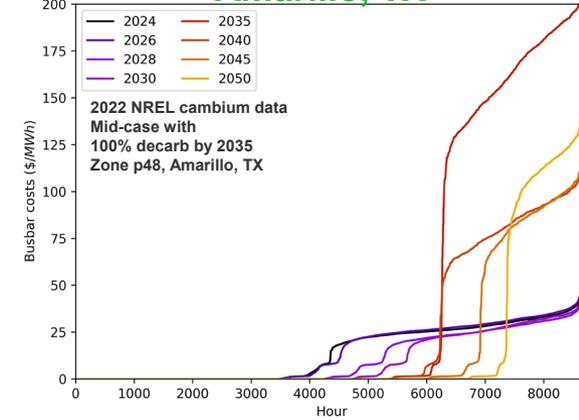
2022 NREL cambium data
Mid-case with
100% decarb by 2035
Zone p48, Amarillo, TX

- We have expanded our analyses to explore "projected" electricity costs.
- We have chosen select locations to highlight the impact of grid mixes.
- Price structures directly influence optimal operating strategies.
- Explores the impact of "chasing" cheap electricity.
- Ignores the impact that electrolysis can have on electricity price structure.

- Full impact of start-up/shutdown on durability is unknown, avoiding shutdown events is possible by staying on and going to lower operating level.

- Lowest operating level achievable to rated power is termed idle state.

- Idle state is ratio of minimum operating power density to rated power density, set by safety/operating limitations.

- Optimum HLC is strong function of turndown and minimum HLC achieved for systems capable of achieving smallest turndown.

Legend:
- Baseline on/off
- 2.5% turndown
- 10% turndown
- 20% turndown

PRELIMINARY

2022 NREL cambium data
Mid-case with
100% decarb by 2035
Year 2030 marginal costs
Zone p28, Palo Verde, AZ

Axis labels: Hydrogen levelized cost ($/kg) vs. Hours operated at full H_2 output (hrs/yr)
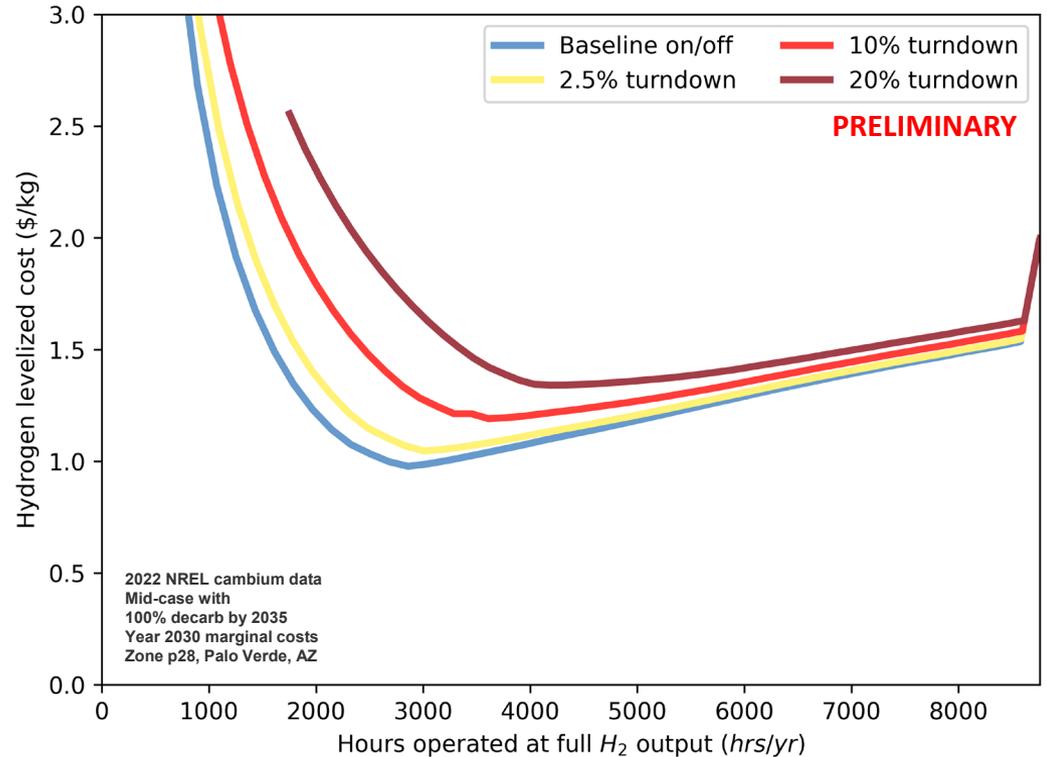
Badgett A, Saha P, Brauch J, Pivovar B. SUBMITTED: Decarbonization of the electric power sector and implications for low-cost hydrogen production from water electrolysis 2023;Advanced Sustainable Systems.

Low Temperature Electrolysis (LTE)

Task 1: Durability (more content in AMR Poster P196a)

1.523 V Upper Potential Limit (equivalent to 2V iR-corrected in FuGeMEA); 1 mV/s

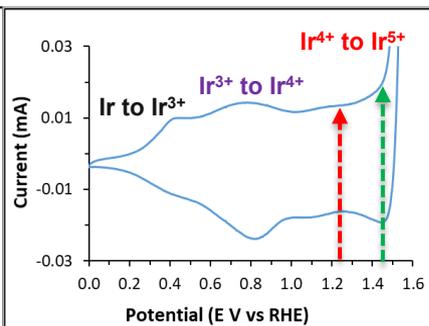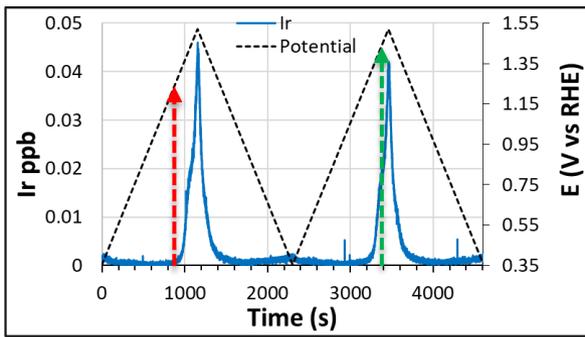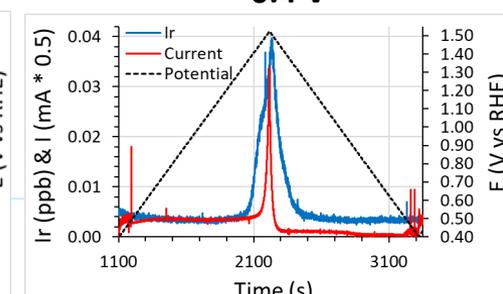**Electrochemical flow cell coupled with ICP-MS. 0.1 M HClO$_4$ electrolyte.**
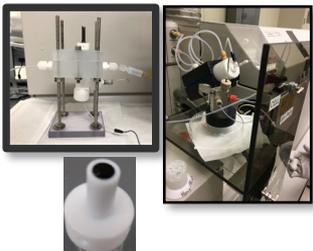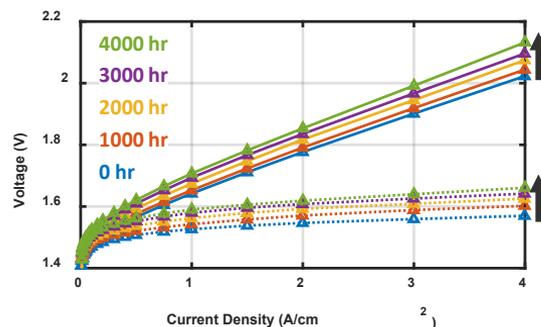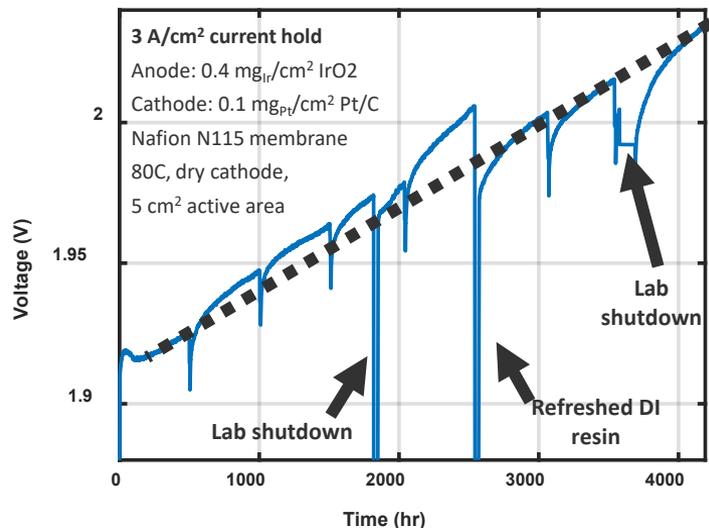
Lower Limit: 1.4 V
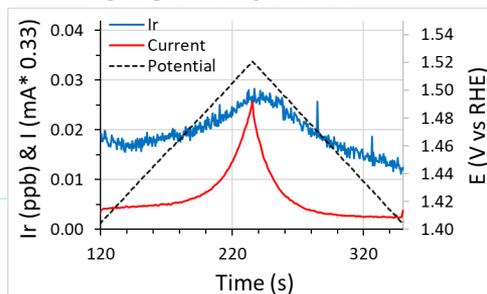
0.8 V
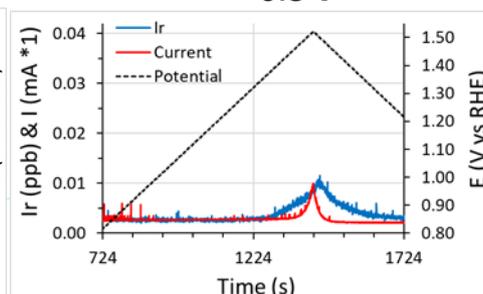
0.4 V

- Alfa Aesar IrO$_x$ is stable at potentials between 0.35 V and ~1.25 V
- Onset of Ir dissolution is at 1.25 V, coinciding with oxidation of Ir^{4+} to Ir^{5+} (determined using in situ X-ray absorption spectroscopy)
- Sharp increase in dissolution at >1.45 V coinciding with onset of OER
- Ir dissolution **during positive potential sweep** decreases with decreasing lower limit of sweep to 0.8 V and increases when lower limit is 0.4 V
- Indicates that increased degradation of Ir during start up-shut down cycling is not caused by dissolution of Ir metal, but by increased dissolution during Ir oxidation

3 A/cm² current hold
Anode: 0.4 mg$_{Ir}$/cm² IrO2
Cathode: 0.1 mg$_{Pt}$/cm² Pt/C
Nafion N115 membrane
80C, dry cathode,
5 cm² active area

Lab shutdown

Refreshed DI resin

Completed 4,000 hr durability test of FuGeMEA cell:

- Benchmarking decay rates:
  - ~28 μV / hr at 3 A/cm²
    - ~ 7 μV / hr ohmic, 21 μV$_{HFR-free}$ / hr
    - Slower decay of ~ 11 μV$_{HFR-free}$ / hr at 0.1 A/cm²
- Understanding mechanisms of steady-state degradation:
  - Catalyst activity or surface area loss
  - Increasing catalyst layer resistance
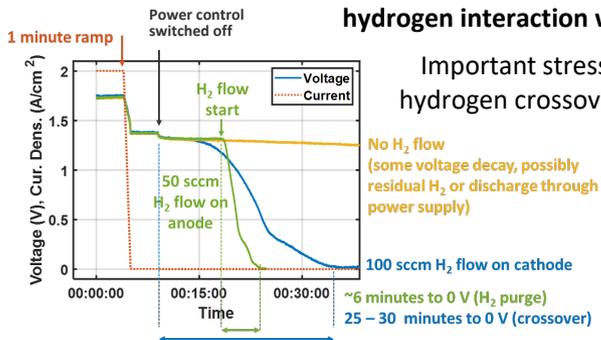 - Possible cation contamination
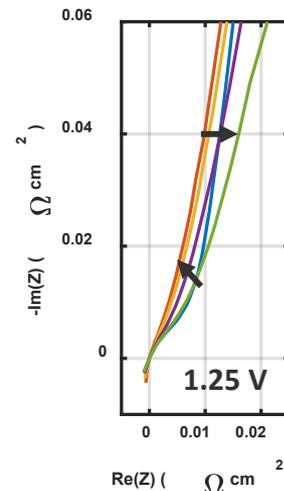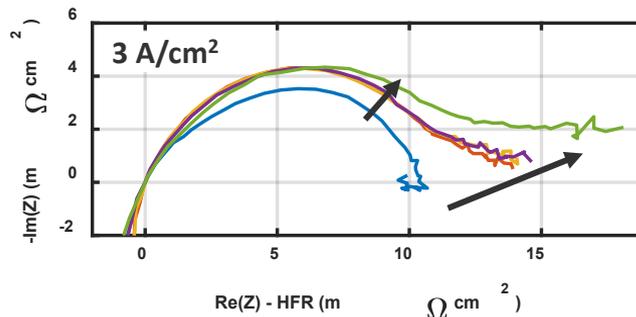
Post-mortem characterization underway to inform mechanistic understanding.

Different Depolarization Behavior Depending on Shutdown Conditions

Slow depolarization (minutes) caused by hydrogen interaction with the anode

1 minute ramp
Power control switched off
H₂ flow start
50 sccm H₂ flow on anode
Voltage / Current

No H₂ flow (some voltage decay, possibly residual H₂ or discharge through power supply)

100 sccm H₂ flow on cathode
~6 minutes to 0 V (H₂ purge)
25 – 30 minutes to 0 V (crossover)

Important stressor to anode from hydrogen crossover during shutdown

No Protective Current
Voltage / Current

Fast depolarization (seconds) caused by rapid current stepping (possible capacitive effect)

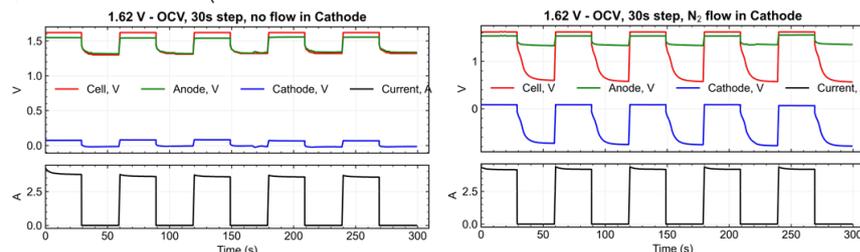Mechanisms must be understood and controlled to design ASTs and mitigation strategies.
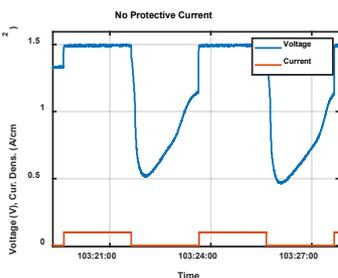
Reference Electrode for Understanding Stressors on Each Electrode

Reference electrode is an essential tool for monitoring anode and cathode states

Flow field plate | Fuel | Gasket | Hydrogen | Reference electrode
Anode
Membrane
Cathode
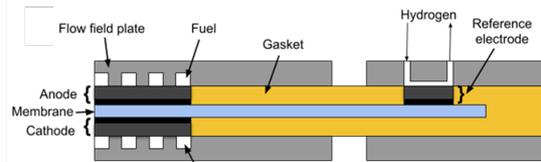
On/Off current cycling without hydrogen on cathode causes cathode potential to change.

1.62 V - OCV, 30s step, no flow in Cathode
Cell, V | Anode, V | Cathode, V | Current, A

1.62 V - OCV, 30s step, N₂ flow in Cathode
Cell, V | Anode, V | Cathode, V | Current, A

[1] Abdelrahman, M. E. et al. Electrochimica Acta 416 (2022): 140262.

Potential on both electrodes can change during shutdown, creating different stressors depending on conditions.

Understanding and controlling different shutdown stressors is key focus for ongoing work to create targeted, reproducible durability tests

- Higher cycling frequency
  - Relevant to increasing loss rate, consistency in mechanism; Concerns at cycle time below 10 s with load stabilization, reproducibility

- Set of options evaluated for catalyst layer ASTs:
  - HFR-free potential is optimal, capabilities limit implementation
  - Potential based cycling less severe, requires setting other components (more suitable component level AST for comparing catalysts)
  - Current based may be more field test relevant, heavily affected by manufacturing and catalyst layer properties (More suitable for MEA level ASTs)

- Forcing anode potential to below Ir redox increases degradation rate

Increasing Cycling Frequency
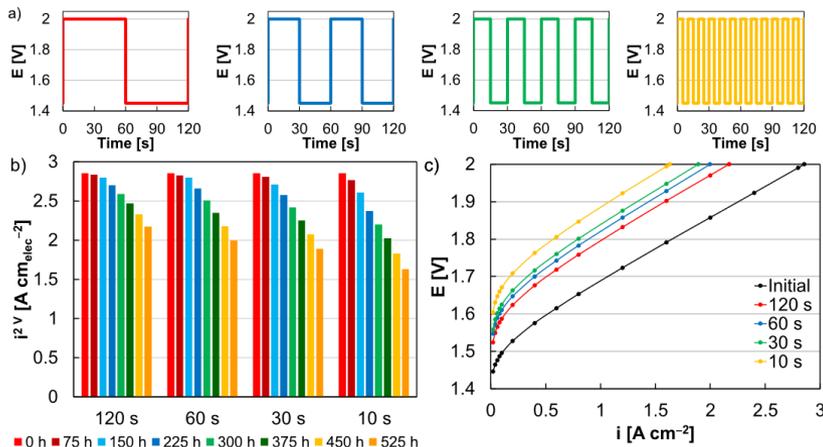
Forcing cell potential to 0.35V

Alia et al. *J. Electrochem. Soc.* **2019**, *166* (15), F1164.
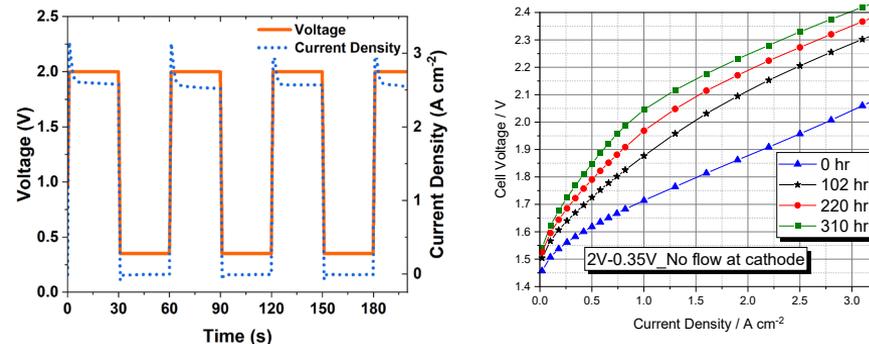
Enhanced degradation rates

Low Temperature Electrolysis (LTE)

**Task 2: Performance and Benchmarking (more content in AMR Poster P196b)**

Accomplishments – Established Methodology for Reproducible Cross-lab Benchmark Performance

- Evaluating progress in cell performance and durability toward Hydrogen Shot targets requires reproducible polarization curves across the LTE labs

- Several test iterations dramatically improved comparability across consortium labs using traveling cell hardware

- Improvement from 200 mV variation down to 4 mV
  - ✓ Removal of water quality issues
  - ✓ Protocol expansion to include reconditioning between separate experiments

- In-situ experimental results are fully reproducible across labs

- Successful benchmarking activities with the international community (IEA) achieved ~20 mV variations with cell assembled at each location


200 mV @ 4 A/cm^2

All: 19 mV

All after re-conditioning: **4 mV**
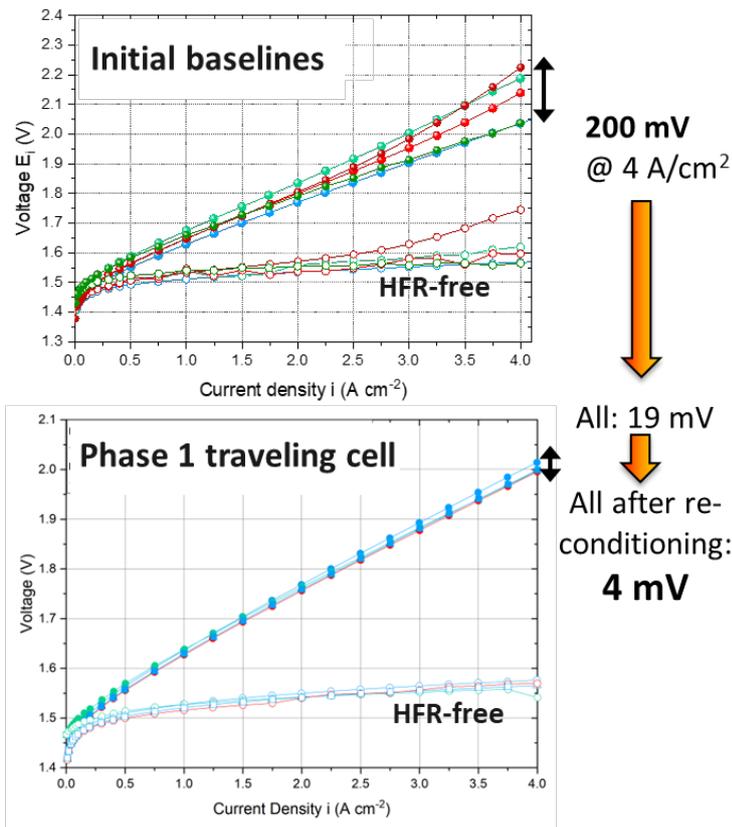
- **Studied impact of differential pressure cycling on ambient pressure VI performance and H_2 crossover**
- **Cell voltage decreased after cell exposure to increasing Δp**
  - ➤ **In contrast to expectations from Nernst equation**
  - ➤ **A second process is occurring**
  - ➤ **We are suspecting a decrease in membrane thickness as cathode pressures force CCM intrusion into the PTL**


Pressure cycle test plan
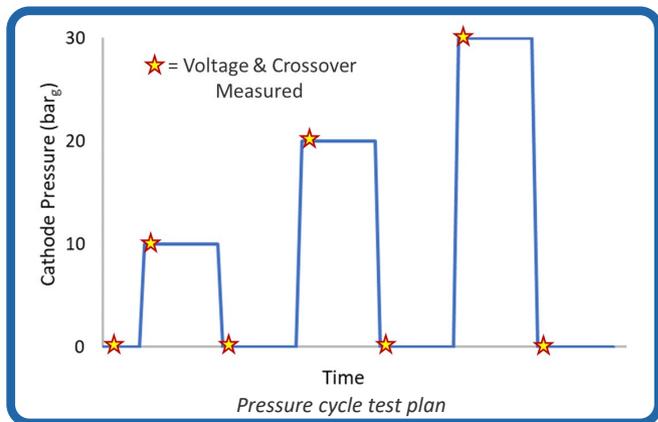
- **H_2 crossover increases dramatically after exposure to elevated pressures**
  - ➤ **This supports the membrane thinning theory**
- **Future work will include EIS to enable a full voltage breakdown analysis**
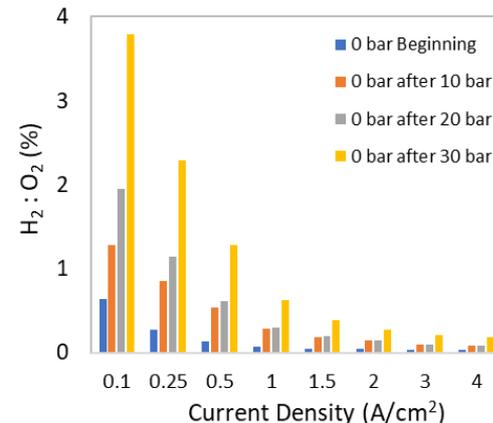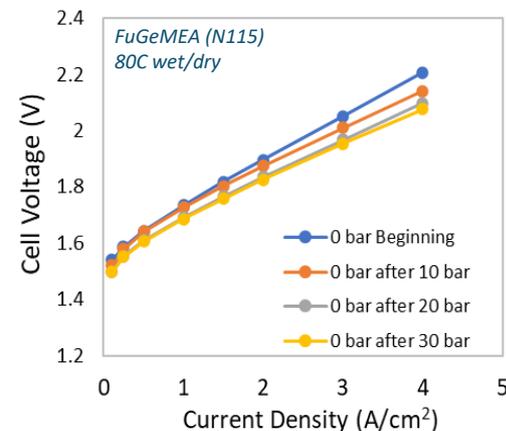
## X-ray Photoelectron Spectroscopy (XPS)
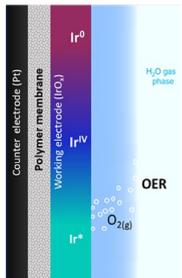
- Operando characterization provides insight into:
  - ✓ Oxidation state of anode catalyst impacting OER activity and degradation processes (XPS, XAFS)
  - ✓ Through plane water distribution impacting cell resistances and transport (Neutron imaging)
- Advanced characterization techniques enable observations of processes within operating electrolyzers and inform model development
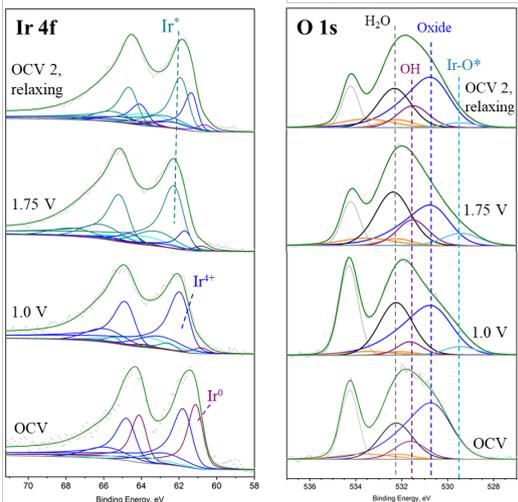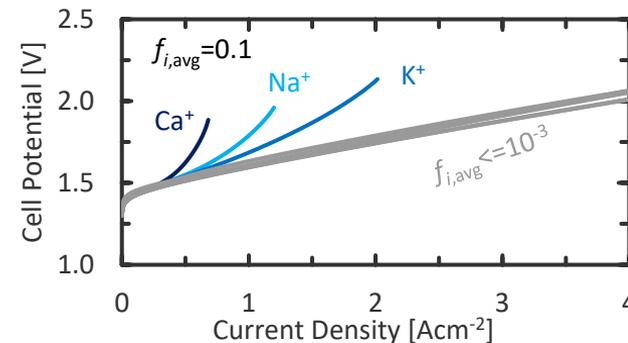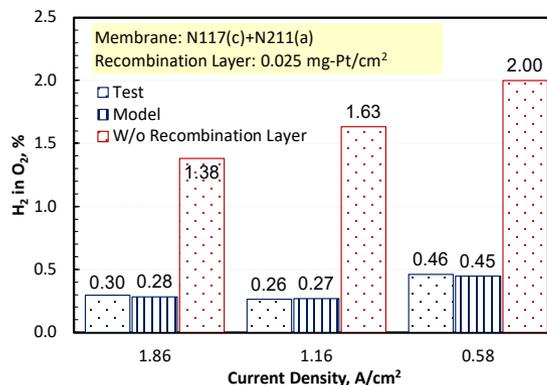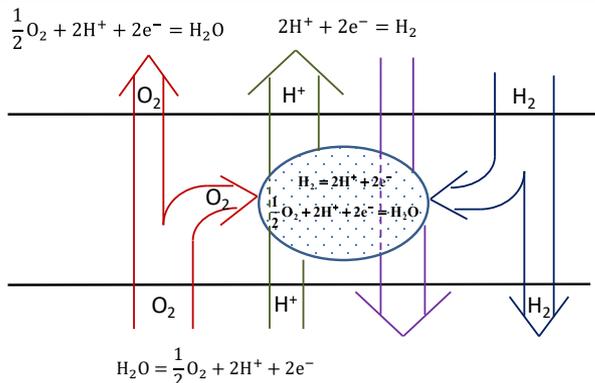

X-ray Absorption Spectroscopy (XAFS)
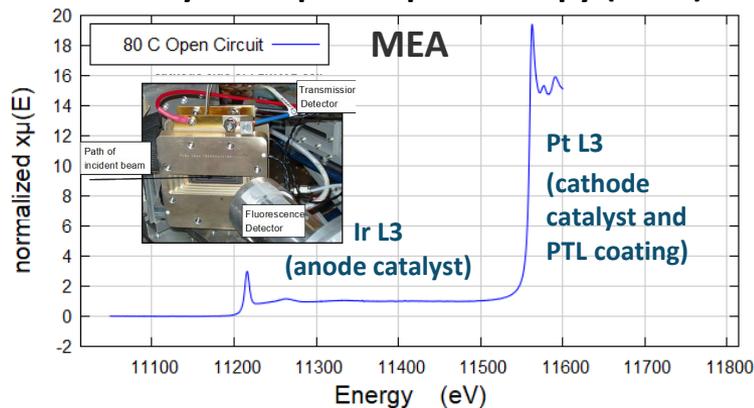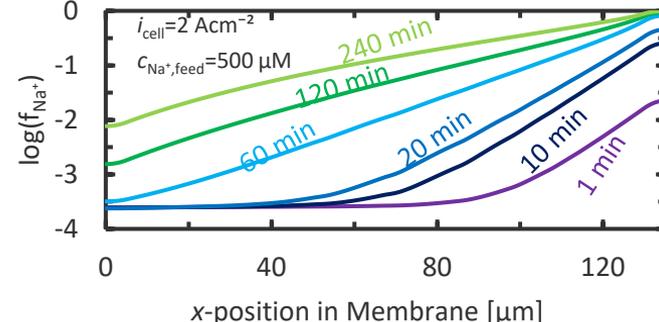

Neutron Imaging (MIT/NIST)
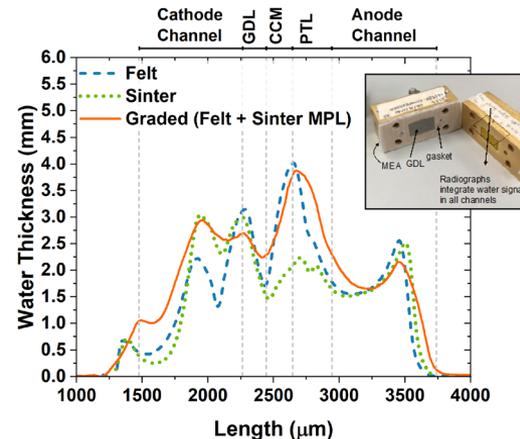
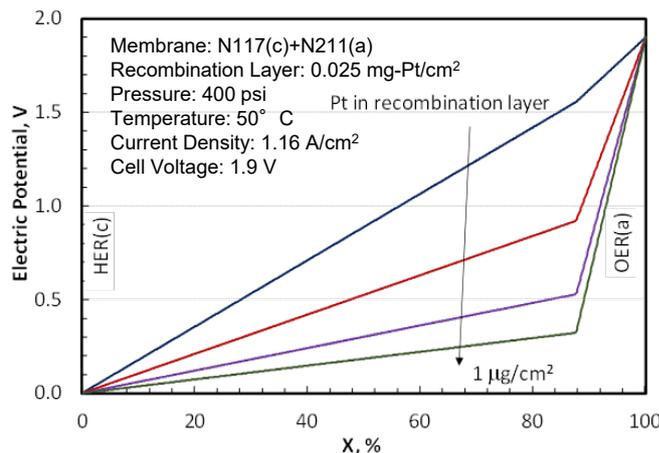# Accomplishments – Developed Models for Hydrogen and Oxygen Crossover and Contaminants

$$\frac{1}{2}O_2 + 2H^+ + 2e^- = H_2O \qquad 2H^+ + 2e^- = H_2$$

$$H_2O = \frac{1}{2}O_2 + 2H^+ + 2e^-$$

- Modeling to inform the recombination layer experimental efforts
- Pt interlayer lowers the electric potential and promotes electrochemical reaction between crossover H_2 from cathode and O_2 from anode.
- Locating the interlayer closer to the anode mitigates H_2 crossover to anode with only a small increase in H_2 crossover from cathode. However, interlayer location may affect Pt stability.

Membrane: N117(c)+N211(a)
Recombination Layer: 0.025 mg-Pt/cm^2

Legend: Test, Model, W/o Recombination Layer

Membrane: N117(c)+N211(a)
Recombination Layer: 0.025 mg-Pt/cm^2
Pressure: 400 psi
Temperature: 50°C
Current Density: 1.16 A/cm^2
Cell Voltage: 1.9 V

Pt in recombination layer

1 µg/cm^2

$f_{i,avg}=0.1$

$f_{i,avg}<=10^{-3}$

Steady-state polarization curves. f_i is the fraction of cation-exchanged sulfonic acid sites. Three cations were simulated Na$^+$, K$^+$, and Ca^{2+}.

$i_{cell}=2$ Acm^{-2}
$c_{Na^+,feed}=500$ µM

240 min, 120 min, 60 min, 20 min, 10 min, 1 min

Cation content as a function of position in the membrane with elapsed exposure time to 500 µM Na$^+$ feed as a parameter at 2 Acm^{-2}.
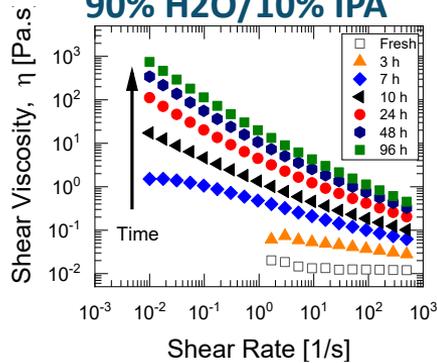
Low Temperature Electrolysis (LTE)

Task 3: Manufacturing, Scale-up and Integration (more content in AMR Poster P196c)

Accomplishment: Shelf-stability of Catalyst Inks

Studies performed to characterize properties of catalyst inks and electrodes as ink ages

Inks:

90% H2O/10% IPA

**Electrodes from:**

50% H2O/50% NPA
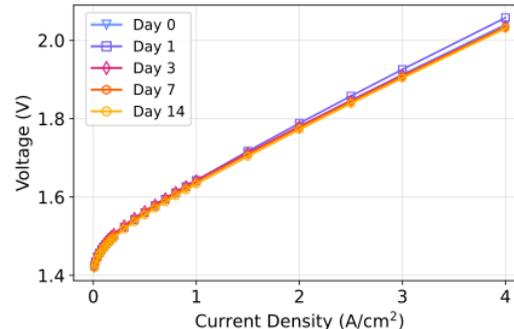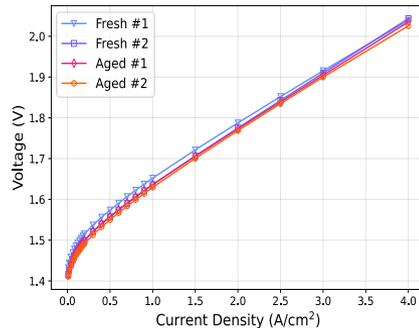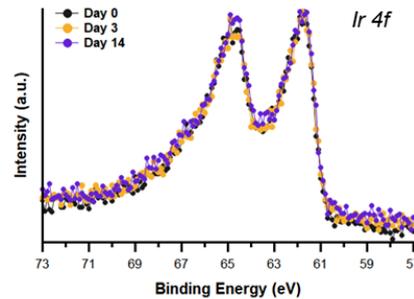
- Water-rich ink (90wt% water) shows dramatic thickening with aging

- XPS shows no change in iridium bonding

- **Most significantly, aged inks perform the same as fresh inks demonstrating shelf-stability**

Accomplishment: Impact of Coating Method on Durability

- DOE 2030 Goal – 0.125 mg_{PGM}/cm^2
- Conducted testing to understand impacts of coating methods on performance and durability
- Compared spray and R2R gravure at two loadings

Gravure-coated electrodes
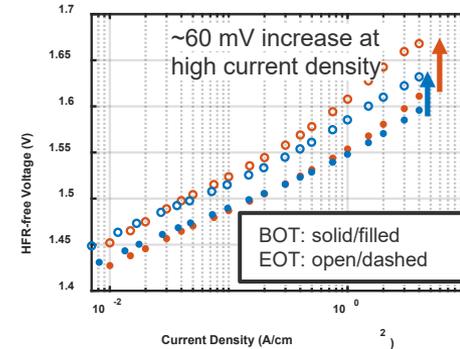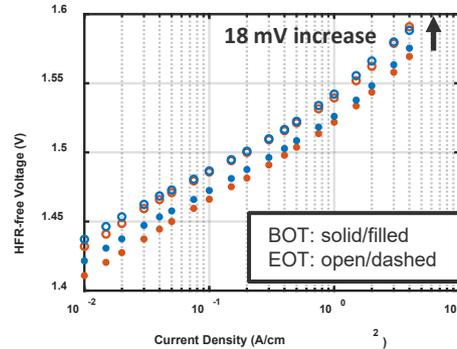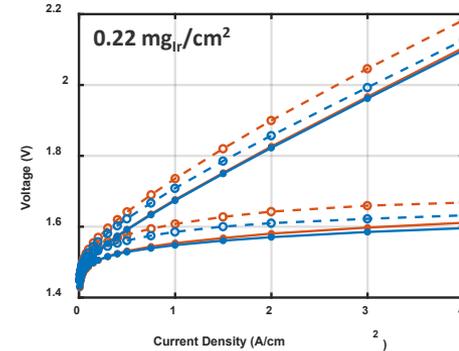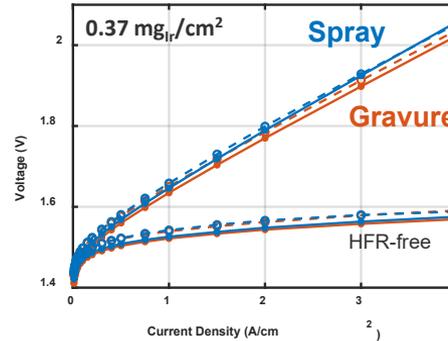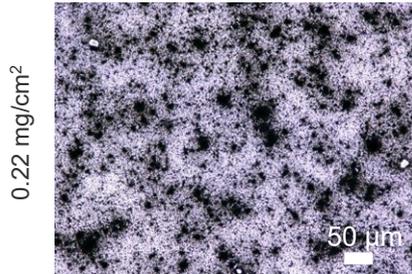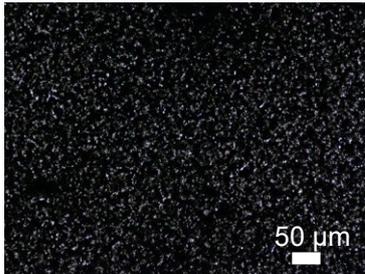
- **CL coating method and homogeneity do not impact initial IV performance**
- **Higher CL heterogeneity not coating method accelerates degradation**

Low Temperature Electrolysis (LTE)

PTLs (Porous Transport Layers)

Cross-task effort (additional information found in Posters 196a, b and c)

Objectives:

- Develop PTLs with optimized structure using scalable processing methods
- Improve understanding of critical structural parameters (pore size, pore shape, pore volume, graded porosity)
- PTL/MPL structures

Accomplishments

- Demonstrated good control of structure via tape casting
- Surpassed performance of baseline commercial PTL

Control of Pore Size with PMMA Porogen

Tomography pore size
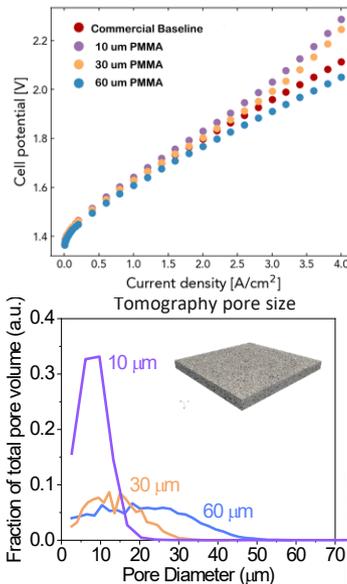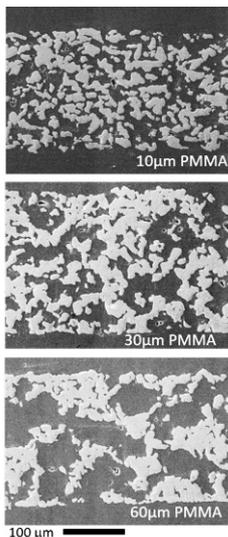
Support/MPL Bilayers

Control of layer thickness

Fine MPL

Fine support

Fine MPL

Coarse support

100μm

Free-standing MPL

Accomplishment: Improving CL/PTL Interface via PTL Surface Modification; Example: Laser Ablation

2GDL10 - 0.25   2GDL5 - 0.125   2GDL3 - 0.15

As-received

300 μm

Laser Ablated

IV Performance

Nafion N117
A: 0.40 mg/cm^2 IrO$_2$
C: 0.1 mg/cm^2 Pt/C
80 °C

Legend:
- 2GDL10-0.25
- 2GDL5-0.125
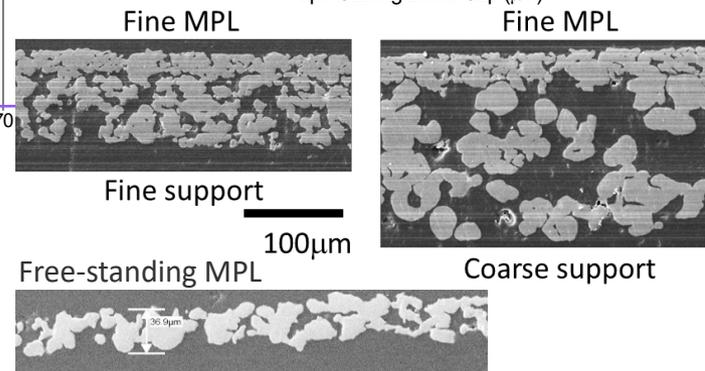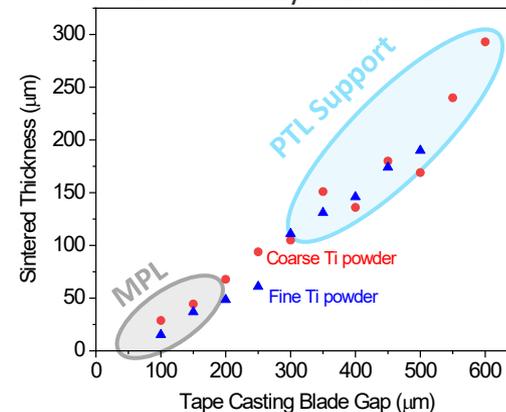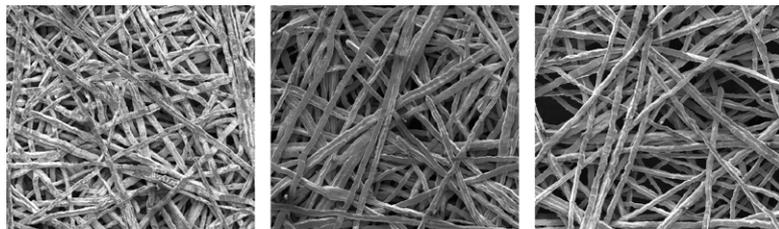- 2GDL3-0.15
- 2GDL10-0.25-Laser
- 2GDL5-0.125-Laser
- 2GDL3-0.15-Laser
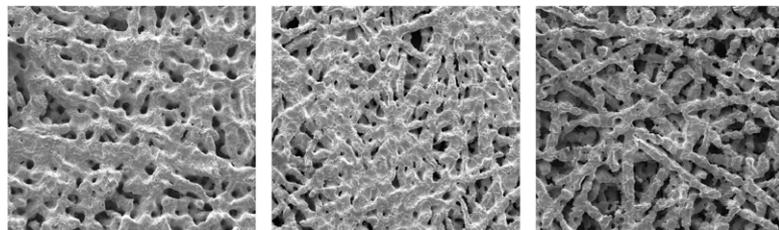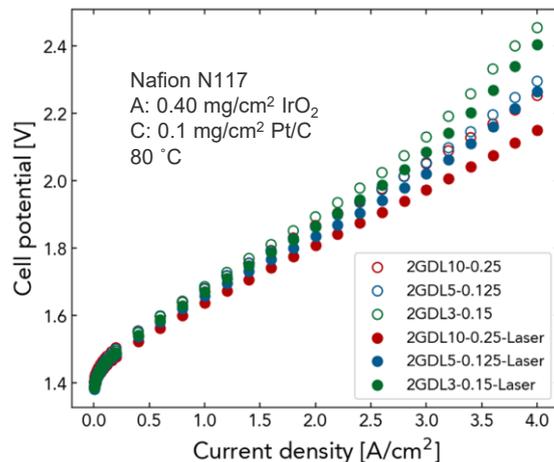
- Investigated use of laser ablation to improve CL/PTL interface and impacts on performance and durability

- Laser ablated PTLs show increase in the measured double layer capacitance, indicating larger ECSA.

- Observed less indentation to the CL/Membrane seed with laser ablated PTLs after AST
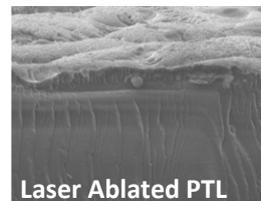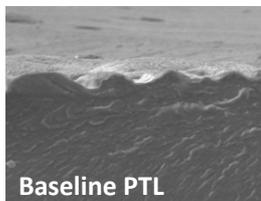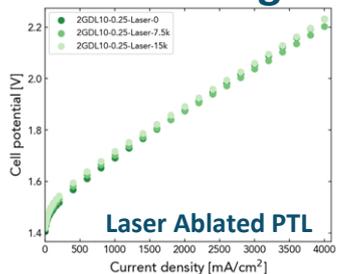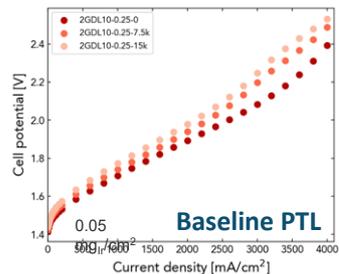
- **Demonstrated that:**
  - **Laser ablation improves Vi performance and durability**
  - **PTL surface abrasions can improve Vi performance**

Accelerated Stress Testing

Baseline PTL

Legend:
- 2GDL10-0.25-0
- 2GDL10-0.25-7.5k
- 2GDL10-0.25-15k

0.05 mg/cm^2

Laser Ablated PTL

Legend:
- 2GDL10-0.25-Laser-0
- 2GDL10-0.25-Laser-7.5k
- 2GDL10-0.25-Laser-15k

Baseline PTL   **Laser Ablated PTL**

10 μm

Accomplishment: Characterized the Effects of PTL Morphology
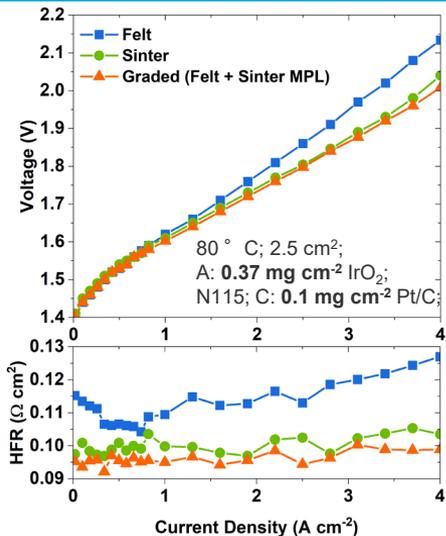
- **Performance of cell with microporous layer (MPL) on PTL is higher due to better contact with anode catalyst layer**

- **Hierarchical structure of PTL with MPL provides better water management**

- **Able to compare same PTL with neutrons and X-ray imaging**

Water thickness from neutron Imaging at 2 A cm⁻²
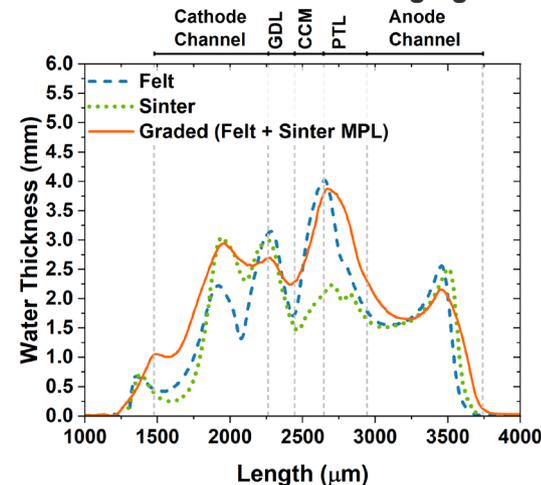
PTL	Thickness (µm)	Porosity	Average Pore Size (µm)
Felt	~240	0.67	15.40
Sinter	280	0.37	4.90
Graded	240+60	0.67+0.40	15.40 + 3.97

O₂ saturation from X-Ray Imaging at 2 A cm⁻²
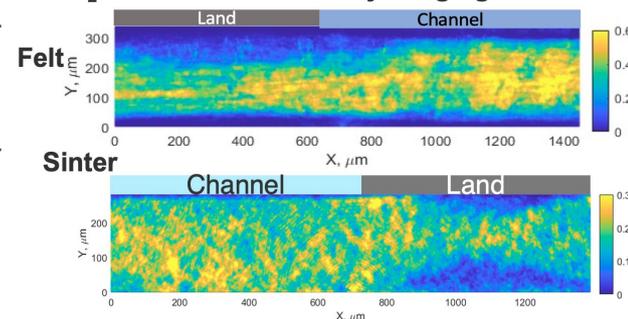
- **Combination of operando Neutron and X-Ray imaging to study O₂ bubble in PTL and water distribution across the MEA.**
- **Future Work: Ex-situ and operando characterization of new PTLs (laser modified, PTLs with MPL, PTLs graded porosity) being studied in H2NEW**

H2NEW Activities: Low Temperature Electrolysis (LTE)

Liquid Alkaline (more content in AMR Poster <u>P196h</u>)

Liquid Alkaline Water Electrolysis

- Mature Technology? Yes, but …
  - Designed for 24/7 steady-state operation
  - Dynamic operation challenges significant (needed for low-cost electrons/energy systems integration)
  - Power density low (turndown capability limited)
  - Degradation not understood, particularly under dynamic operation

- Research needs
  - Reproducibility / Benchmarking
  - Explore optimized operating strategies, quantify durability impacts
    - ✓ Maximum/minimum operating conditions (turndown capability limit key concern for economics)
    - ✓ Impact/ability to tolerate start-up/shut-down
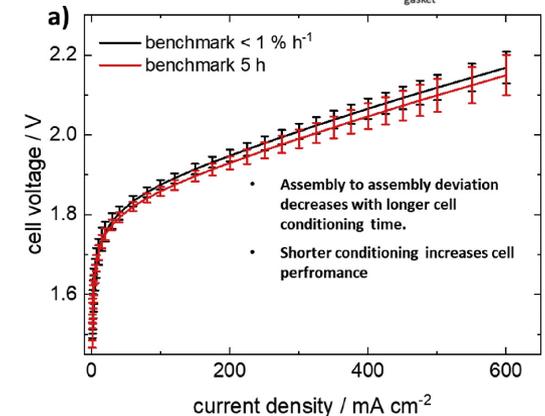 - Achieve higher operating current density (lower cell resistance, engineered separator)
  - Reduce minimum turndown (gas crossover reduction, engineered separator)
  - Improve efficiency (improved catalysis, engineered separator)
  - Improve durability (mitigation strategies)
  - Increased pressure operation (cell operating strategy, engineered separator)
  - Systems and Techno-economic Analysis (system design, operating strategy, hydrogen levelized costs)

C. Karacan et al., Intern. J. of Hydrogen Energy 47 (2022) 4294

Accomplishments : Reference Liquid Alkaline Water Electrolysis (LAWE) System

> ➢ **Develop reference system configurations for performance, durability and cost studies**
>
> ➢ **Develop quantitative understanding of mechanisms that determine system dynamic response to load changes, turndown, efficiency at rated power and partial loads, and durability.**

Distributed LAWE System

1. Electrolyzer Stack
- MEA
  Separator: ZrO_2 Diaphragm (Zirfon)
  OER Anode Catalyst: Raney Ni (Ni-Al)
  HER Cathode Catalyst: Mo-doped Raney Ni (Ni-Al-Mo)
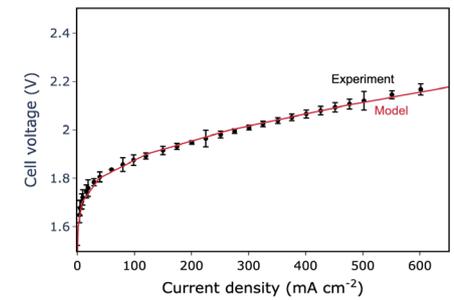 Electrode Substrate: Ni-coated Expanded SS Sheet
- Anode O_2 PTL: Sintered Porous Ni
- Cathode H_2 PTL: Sintered Porous Ni
- Bipolar Plates: Ni Coated SS
- Current Collectors: Ni Coated Expanded SS
- End Plates: SS

2. Electrical BOP System
- Transformer
- Rectifier

3. Feed Water System
- Feed Pumps
- Water Purification Plant
- Water Reservoir

4. KOH System
- KOH Recirculation Pump
- KOH Cooler

5. Gas Treatment System
- Anode H2-Water Separator
- H2 Cooler
- H2 Scrubber
- Cathode O2-Water Separator
- O2 Cooler

6. H_2 Purification System
- H_2 Buffer
- H_2 Compression Unit
- Deoxidizer
- Condenser
- H_2 TSA Dryer

7. Cooling Water System
- Compression Chiller
- Dry Cooler

Centralized LAWE System

1. Stack Modules
  1.1 4 X 2.5 MW stacks
  1.2 Electrical BOP Subsystem
  1.3 KOH Subsystem
  1.4 Gas Treatment Subsystem
2. High Voltage Transformer
3. Feed Water System
4. H_2 Purification System
5. Cooling Water System

M Holst, S Aschbrenner, T Smolinka, C Voglstätter, G Grimm, COST FORECAST FOR LOW TEMPERATURE ELECTROLYSIS – TECHNOLOGY DRIVEN BOTTOM-UP PROGNOSIS FOR PEM AND ALKALINE WATER ELECTROLYSIS SYSTEMS, Fraunhofer Institute for Solar Energy Systems ISE, Oct 2021

H2NEW
U.S. DEPARTMENT OF ENERGY

Serpentine flow plates

30 wt% KOH

$2OH^- \rightarrow 2e^- + H_2O + \frac{1}{2}O_2$

O_2

Heating element

OH$^-$

30 wt% KOH

$+ 2e^- \rightarrow H_2 + 2OH^-$

H_2

O_2

30 wt% KOH

Ni anode	Agfa Zirfon separator	Ni cathode
300 μm	500 μm	300 μm

H_2

30 wt% KOH

- Utilize physics-based cell modeling to understanding limiting phenomena and be able to conduct sensitivity studies

Experiment / Model — Cell voltage (V) vs Current density (mA cm^{-2})

Applied Voltage Breakdown

Mass transfer; Kinetics – cathode; Kinetics – anode; Ohmic – cathode; Ohmic – anode; Ohmic – separator

$$\nabla \cdot n_i = \varepsilon_I \sum_i R_{k,i}$$

$$n_i = -D_i^{eff}\nabla c_i + z_i \frac{F}{RT}D_i^{eff}c_i\nabla\phi_I$$

$$\sum_i z_i c_i = 0$$

$$\nabla \cdot i_s = -\nabla \cdot (\sigma_{eff}\phi_s)$$

Bubble coverage

$$a_v = a_v^0(1-\theta)$$

$$\theta = 0.023 i_{total}^{0.3}$$

$$R_{B,i} = M_i \sum_i s_{i,n}(k_n \prod_{s_{i,n}<0} c_i^{-s_{i,n}} - \frac{k_n}{K_n}\prod_{s_{i,n}>0}c_i^{s_{i,n}})$$
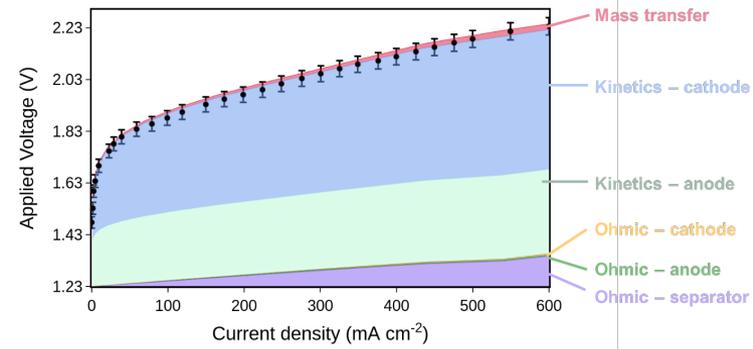
$$R_{CT,i} = -M_i\frac{a_v s_{i,k} i_k}{n_k F}$$

$$i_{HER,base} = -i_{0,HER,base}\ exp\left(-\frac{\alpha_{c,HER}F}{RT}\eta_{HER}\right)$$

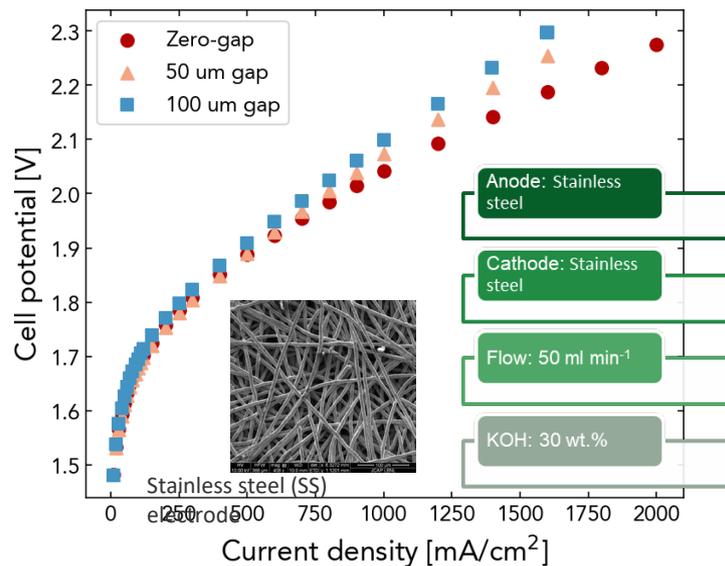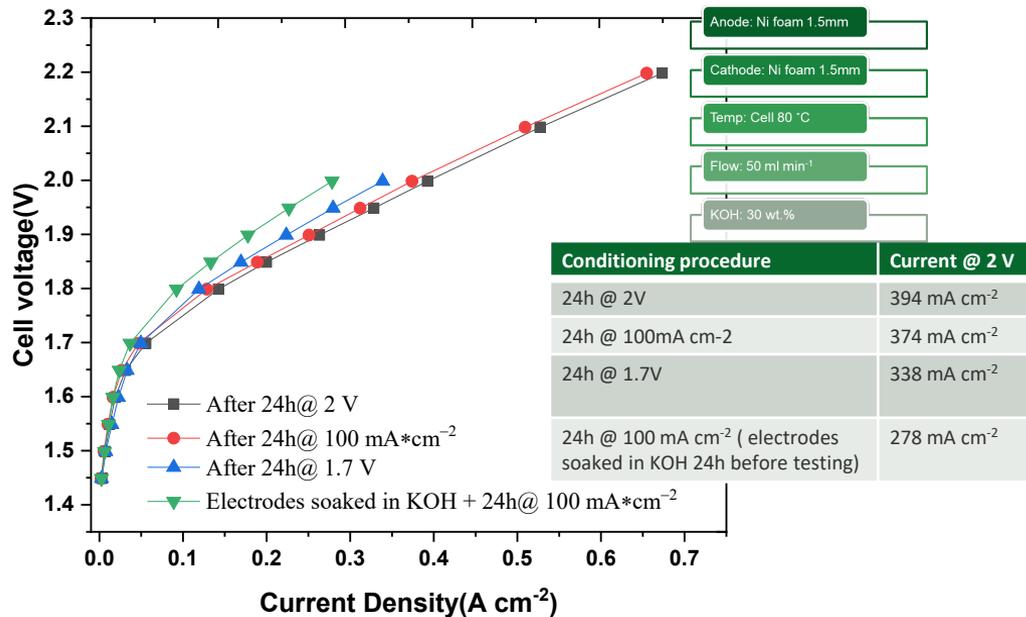$$i_{OER,base} = i_{0,OER,base}\left(\frac{c_{OH^-}\gamma_{OH^-}}{1\ [M]}\right)exp\left(\frac{\alpha_{a,OER}F}{RT}\eta_{OER}\right)$$

$$\eta_k = \phi_s - \phi_l - \left(U_k^0 - \frac{2.303 RT}{F}pH\right)$$

$$pH = -\log K_W - \log\frac{a_W}{\gamma_{OH^-}m}$$

Anode: Ni foam 1.5mm
Cathode: Ni foam 1.5mm
Temp: Cell 80 °C
Flow: 50 ml min⁻¹
KOH: 30 wt.%

Conditioning procedure	Current @ 2 V
24h @ 2V	394 mA cm⁻²
24h @ 100mA cm-2	374 mA cm⁻²
24h @ 1.7V	338 mA cm⁻²
24h @ 100 mA cm⁻² (electrodes soaked in KOH 24h before testing)	278 mA cm⁻²

Anode: Stainless steel
Cathode: Stainless steel
Flow: 50 ml min⁻¹
KOH: 30 wt.%

Stainless steel (SS) electrode

- ➢ It is of utmost importance that a stable cell condition is established prior to performance testing.

- ➢ The effects of the conditioning process are essential to understanding the electrodes, separator, and cell performance.

- ➢ Finite-gap underperform even with very small gap due to increased HFR especially at high currents

- ➢ **Regulating bubble transport pathway will be a potential method to improve finite-gap performance**
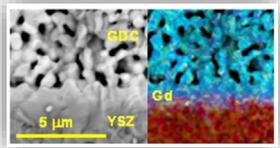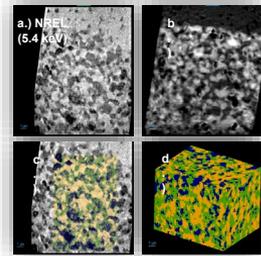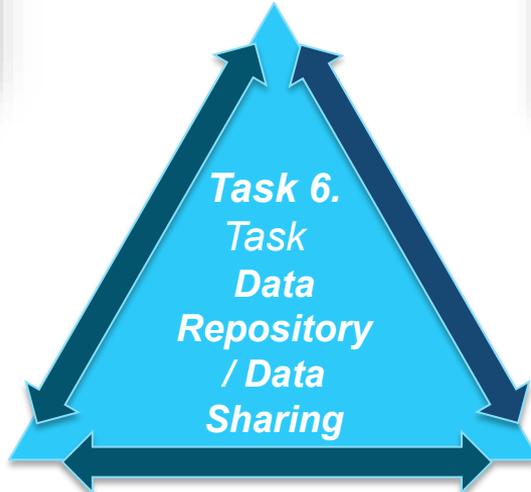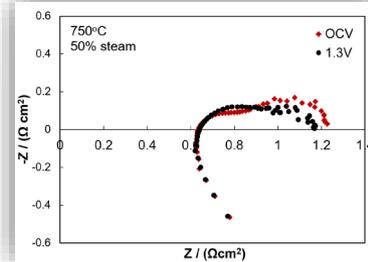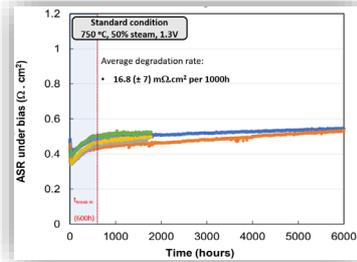
H2NEW Activities: High Temperature Electrolysis (HTE)
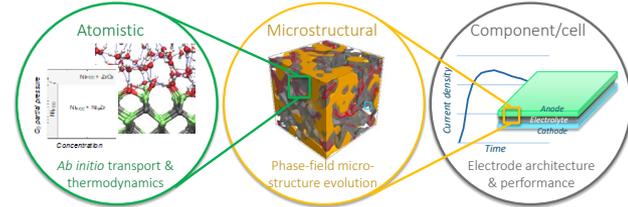
Richard Boardman, H2NEW Deputy Director, and HTE Lead

Approach: High Temperature [Steam] Electrolysis: o-SOEC
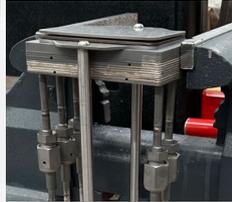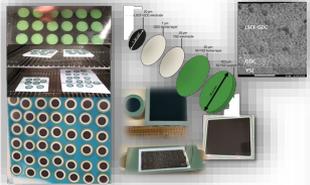
**Task 5.
Cell Accelerated Stress Testing and Measurements**

**Task 6.
Task Data Repository / Data Sharing**

**Task 7.
Characterization:
Cell and Materials Analysis**

**Task 8.
Multi-Scale
Degradation Modeling**

Multiscale physics-based modeling of mechanisms

Atomistic — *Ab initio* transport & thermodynamics

Microstructural — Phase-field micro-structure evolution

Component/cell — Electrode architecture & performance

Relevance: HTE Path to DOE hydrogen cost goals.

- ❑ **Reduce systems/balance of plant costs**
  - ▪ Lower operating temperature
  - ▪ Reduce oxygen-sweep
  - ▪ Increase external heating source
  - ▪ Optimize systems design and operations
  - ▪ Maximize plant scale
- ❑ **Reduce stack manufacturing costs**
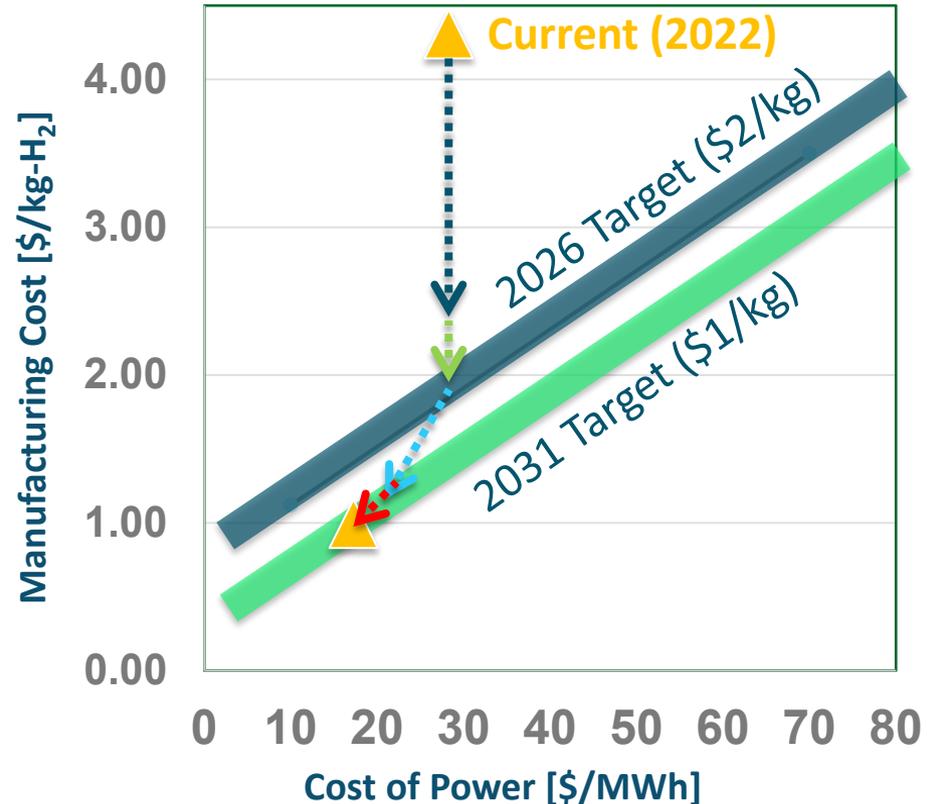- ❑ **Increase stack efficiency**
  - ▪ Increase steam conversion efficiency
  - ▪ Reduce ohmic heating by reducing area-specific resistance
  - ▪ Increase area-specific Faradaic efficiency by increasing current density
- ❑ **Increase stack endurance (>60,000 hr)**
- ❑ **Couple with industrial process**
  - ▪ Heat source (e.g., ammonia or fuels synthesis
  - ▪ Replacement of air-separation unit for O_2

Nth-of-a-Kind, 100 - 1000 MWe HTE

Chart: Manufacturing Cost [$/kg-$H_2$] vs Cost of Power [$/MWh], showing Current (2022), 2026 Target ($2/kg), and 2031 Target ($1/kg).

Approach: Select HTE Milestones*

Milestone Name/Description	Due Date	Type	Status
Stack test stand check (including power, hydrogen and steam supply, connection, etc), and test protocol finalization and get the concurrence from the Nexceris team. (INL, NETL)	12/31/2022	QPM	Complete
Complete inter lab button cell performance validation using benchmarking protocols: obtain I-V and EIS data and compare the degradation rate reproducibility equivalent to a standard deviation of 20%. (PNNL, LBNL)	12/31/2022	QPM	Complete
Identify priority samples for testing, analysis, and characterization in order to inform and validate modeling activities. (LLNL, NETL, LLNL, NREL, PNNL)	12/31/2022	QPM	Complete
Develop advanced electrical waveform technique for interrogation of button cells. (INL,NETL) Steam cycling frequency testing and power cycling testing (LBNL)	3/31/2023	QPM	Complete
Modify HydroGEN/H2NEW data hub to facilitate data sharing. Create a datahub file structure for storing and exchanging of model codes, synthetic microstructures, and simulation data. (NETL, LLNL, NREL, PNNL, INL, LBNL)	3/31/2023	Milestone	Complete
Complete button and planar cell testing as well as cells with symmetrical Ni-YSZ electrodes, under high, 90%+, steam operating conditions. Complete post-test characterization of the Ni-YSZ electrode. (PNNL,NETL)	6/30/2023	Milestone	On Track
Determine if elevated pressure is an effective stressor capable of accelerating degradation of Ni/YSZ and/or LSCF by > 20% and establish effect of steam utilization on the degradation rates. (PNNL) Demonstrate that the calibrated performance model can be used within NETL's performance degradation modeling framework.(NETL, NREL)	9/30/2023	Milestone	On Track

*Partial list, see associated 2023 AMR posters for additional details

Select HTE Highlights

- 2023 AMR Select Highlights
  - Task 5 – Testing & Measurements
    - Established Multiple Size Cell Production
    - Achieved excellent production quality control and consistent testing
    - Established Inter-Lab Standardized Testing Protocol and Operating Procedures
    - Inter-Laboratory cell testing is closing on consistent test outcomes
    - Identified Stressors to Accelerate Degradation Mechanisms
    - Larger cell test stand with realistic interconnects, coatings, and contacts now under testing
  - Task 6b – Data Hub
    - Created Data Hub for H2NEW
    - Roll-out and demonstration, March 2023
  - Task 7 – Advanced Characterization
    - Cell characterization using standard microscopy and state-of-the-art X-ray and electron transmission microscopy.
    - Validated X-ray attenuation predictions and demonstrated XRD can be used to resolve crystal structures and defects from individual layers of intact cells (XRD, right) with simultaneous compositional analysis (XRF, below)
  - Task 8 – Degradation Modeling
    - Assessed impact of Ni/YSZ ration, operating conditions, and microstructure on Ni redistribution
    - Demonstrated multiscale framework for predicting penetration into packed GDC
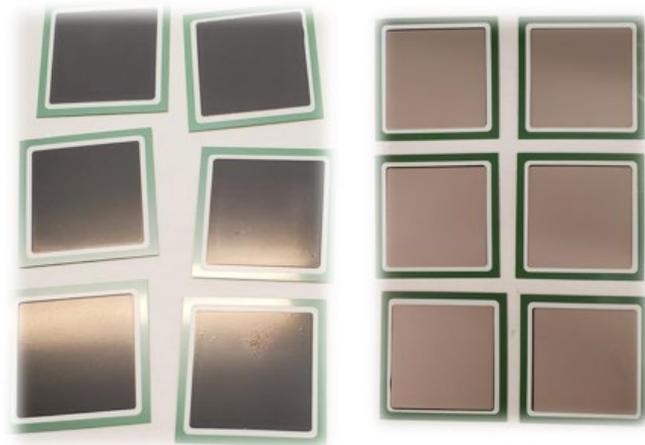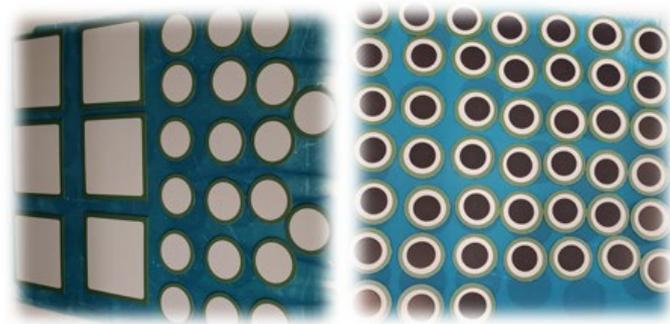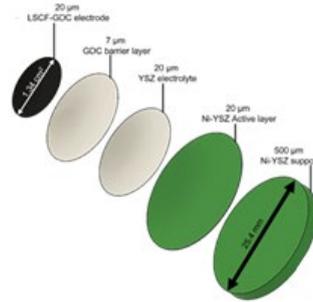   - Ab initio calculation use to parameterize multiscale models

https://www.hydrogen.energy.gov/pdfs/review22/p196_pivovar_boardman_2022_o.pdf

High Temperature Electrolysis (HTE)

Task 5: Durability Testing and AST Development
(more content in AMR Poster P196E, Olga Marina, et al.)
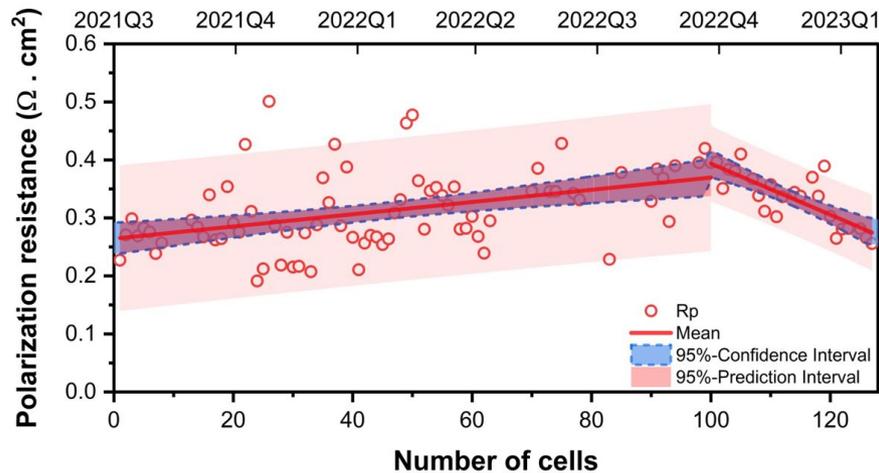
H2NEW
U.S. DEPARTMENT OF ENERGY

- Consortium labs use <u>identical</u> cells for testing, performance validation, and characterization
- Ni-YSZ electrode-supported cells in 4 different formats:
  - 2.5 cm diameter (1-5 cm^2 active area) cells
  - 1-5 cm^2 symmetric cells
  - 4 x 9 cm cells (13 cm^2 active area)
  - 5 x 5 cm cells (16 cm^2 active area)
- A batch fabrication process was developed to minimize the variance between separate cells

Cell performance reproducibility at PNNL

130 different cells tested over period of 20 months using "standard" conditions: 750°C, 1.3V, 50% H_2O

Automation of several fabrication steps and tighter test protocols improved polarization resistance

Ohmic resistance is consistently low

Technical Accomplishment:

Established Inter-Lab Standardized Testing Protocol and Operating Procedures

LSCF electrode paste used to mount platinum mesh current collectors on the oxygen electrode.

Steam/Hydrogen electrode uses nickel paste to mount nickel mesh.

Cell preparation standardization

- Current collectors & attachment
- Precious metal reduction

Cell testing standardization:

- Heat-up
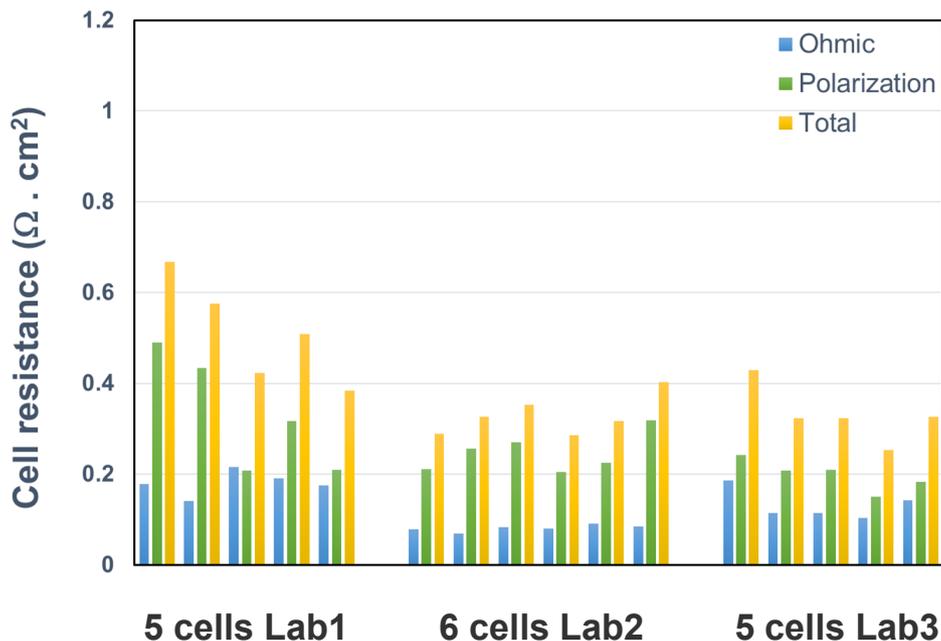- Reduction
- Compositions

Button-Cell
2-4 cm² active area

Enlarged Planar Cell
10-25 cm² active area

Text Parameters

- Temperature
- Voltage & Current Density
- Steam/H2 mixture flow and contact with cell

Benchmarking cell performance and testing protocols

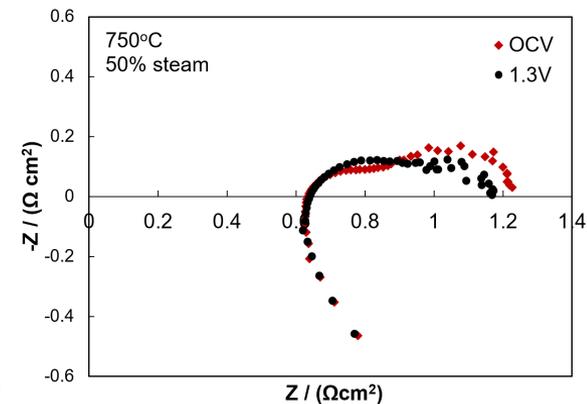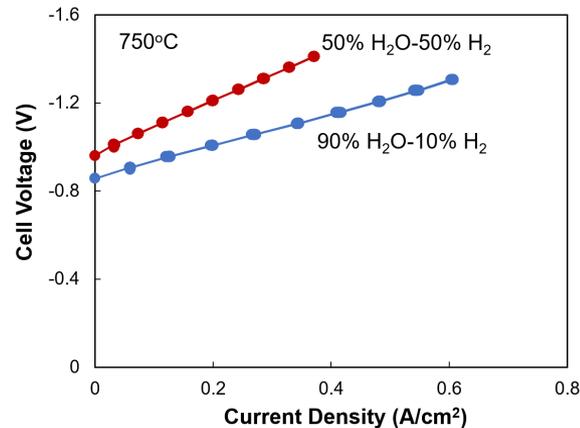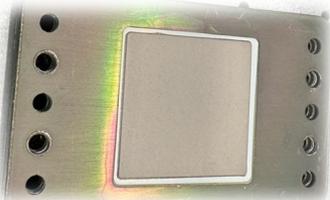|		Intra Lab Reproducibility		
	Ave. Ohmic R ($\Omega.cm^2$)	Std. Error ($\Omega.cm^2$)	Ave. Polarization R ($\Omega.cm^2$)	Std. Error ($\Omega.cm^2$)
LBNL	0.180	0.024 (13%)	0.331	0.115 (35%)
PNNL	0.081	0.007 (8%)	0.248	0.039 (16%)
INL	0.132	0.030 (23%)	0.198	0.031 (16%)
		Inter Lab Reproducibility		
LBNL + PNNL + INL	0.128	0.046 (36%)	0.258	0.088 (34%)

- Observed substantial performance variances between the labs in early testing rounds
- Significantly improved interlab reproductivity by developing standard operating procedures

# of cells	Time (h)	H$_2$O (%)	V (V)	η (V)	T (°C)	Stressor
6	6,000	50	1.3	0.35	750	none
6	3,000	50	1.3	0.35	750	none
3	2,000	50	1.3	0.35	750	none
1	1,000	50	1.3	0.35	750	none
1	2,400	50	1.3	0.35	750	none
2	3,000	50	1.3 → 1.6	0.65	750	V
2	6,000	50	1.3 → 1.5	0.55	750	V
1	1,000	50	1.5	0.55	750	V
1	1,000	50	1.6	0.65	750	V
1	3,000	90	1.3	0.45	750	pH$_2$O
2	2,400	90	1.2	0.35	750	pH$_2$O
2	2,400	10	1.4	0.35	750	pH$_2$O
1	2,400	95	1.175	0.35	750	pH$_2$O
2	1,000	90	1.2	0.35	800	pH$_2$O
2	1,000	10	1.4	0.35	800	pH$_2$O+T
1	1,000	95	1.2	0.35	800	pH$_2$O+T
1	3,000	50	1.3 → 1.5	0.55	800	T, V
2	3,000	90	1.3	0.35	800	pH$_2$O+T
1	3,000	50	1.3 → 1.5	0.55	800	T, V
4	2,000	50	1.3 → OCV	0.35	750	V cycling, different cycling frequency
2	1000	50	1.3 → 0.8	0.35	750	SOFC-SOEC cycling

- Validated seal quality
- Validated ability to produce and deliver 50-90% steam

- Separated ohmic and electrodic losses
- High ohmic losses attributed to poorer contacts compared to button cells

High Temperature Electrolysis (HTE)

Task 7: Advanced Characterization
**(more content in AMR Poster P196e and p196f)**

Characterization

❑ ***Established multi-faceted characterization approach*** across multiple length scales (nm to micron) to elucidate failure mechanisms enabling next generation cell development.

- Characterized cells aged for varying lengths of time and under varying conditions to ***discover trends in degradation*** and evaluate accelerated testing protocols to ensure kinetics, and not thermodynamics, of cell aging are altered.

- ***Integrated characterization*** efforts with ***modeling*** efforts to understand the impact of observed cell degradation on performance.

PNNL Scanning Electron Microscope

NREL, PNNL, INL Advanced CT
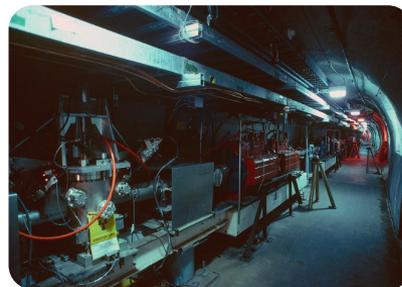
Stanford Linear Particle Accelerator

ANL Advanced Photon Source

Characterization of oxygen electrode and barrier layer – Potential Impact

Highly integrated synchrotron XRD and electron microscopy approach.

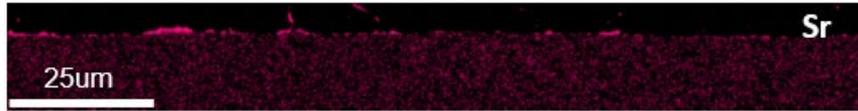| STEM/EDX	Synchrotron XRD
Identifies frequently occurring cation correlations and locations at 1 nm-scale resolution. *XRD results inform TEM what phases are present	Identifies & quantifies all phases present at 1-µm resolution within minutes. *EDX results critical to differentiating between candidate phases w/ identical scattering patterns
Local phase concentrations	Bulk phase concentrations
Cation location within nm-resolution and migration pathways	Phase location with µm-resolution
Sub-nm resolution technique requiring significant sample prep	No sample prep/high throughput/µm-scale technique valuable for statistically relevant results & down selecting cells for further analysis

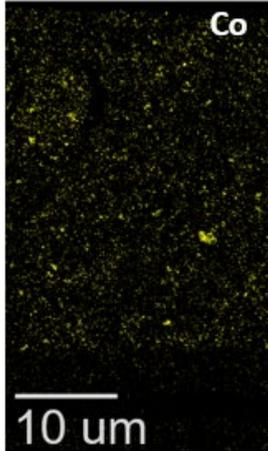## Results are integrated directly into the modeling effort.

Oxygen Electrode Characterization

Elemental maps of Hydrogen Electrode

Sr surface segregation

Dopant in barrier layer migrates into YSZ
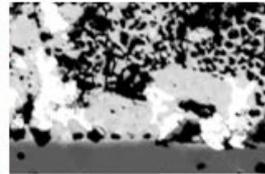
Ag migration into barrier layer and YSZ

Spinel formation increases during testing
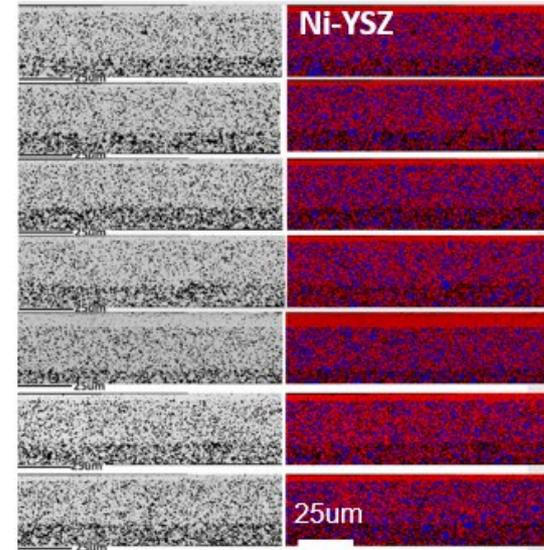
- No obvious Ni migration
- Ni coarsening and Ni – YSZ particle detachment observed in 90-100% steam at 750°C

Accomplishments and progress: Characterization of oxygen electrode and barrier layer

STEM-EDS – Pre Ni Reduction and Testing

- EDS of the oxygen electrode layer reveals initial cation exsolution (predominantly Sr) at the interface and in the barrier layer
- Formation of $CoFeO_x$, SrO, and other phases occur before testing

STEM-EDS – Tested for 1k hrs

- Sr migration through the GDC and accumulation at the YSZ interface occurs
- Increase in $CoFeO_x$ spinel concentration
- GDC breakdown resulation into $CeCoFeO_x$ spinelting in Gd accumulation at the YSZ interface

The oxygen electrode has undesired phases present prior to any ageing; cation migration and degradation increase in severity with cell ageing
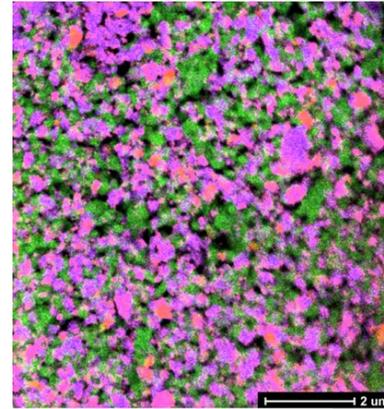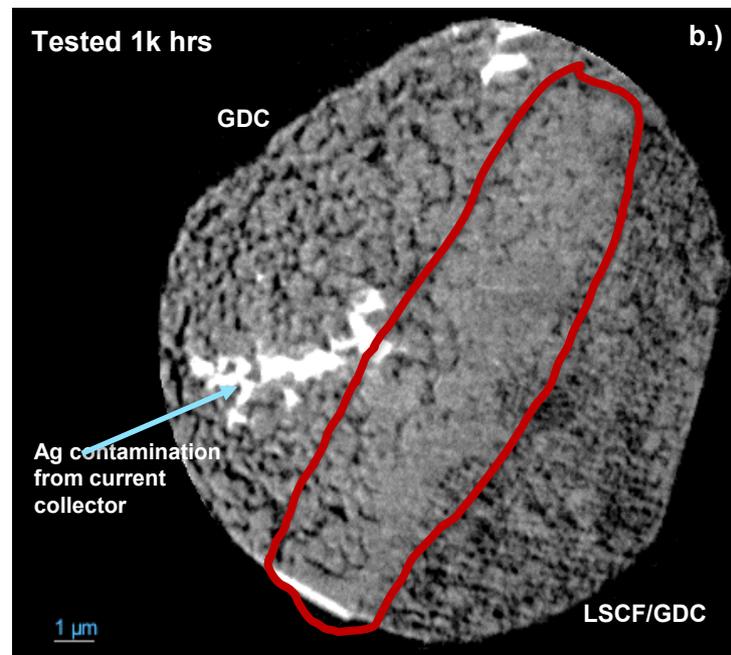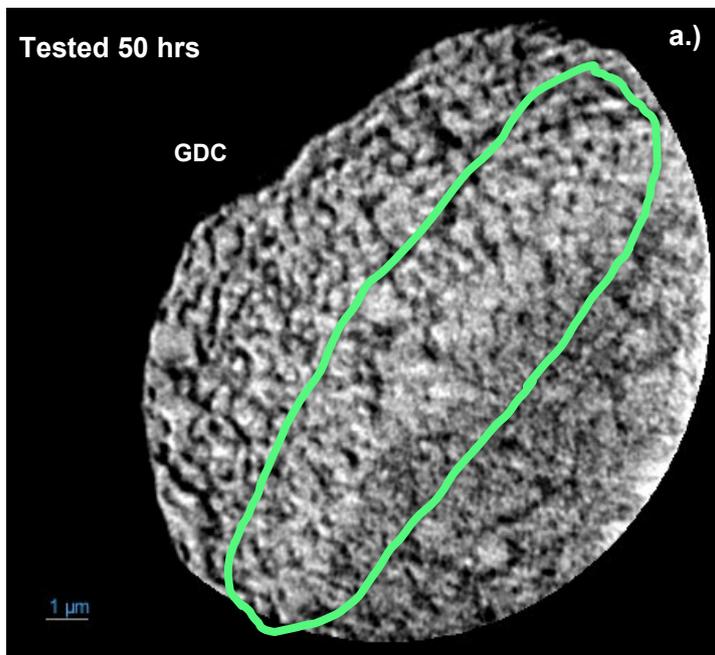

EDS map of Co, Fe, and Ce in the oxygen electrode where $CoFeO_x$ spinel appears pink

Strontium Migration
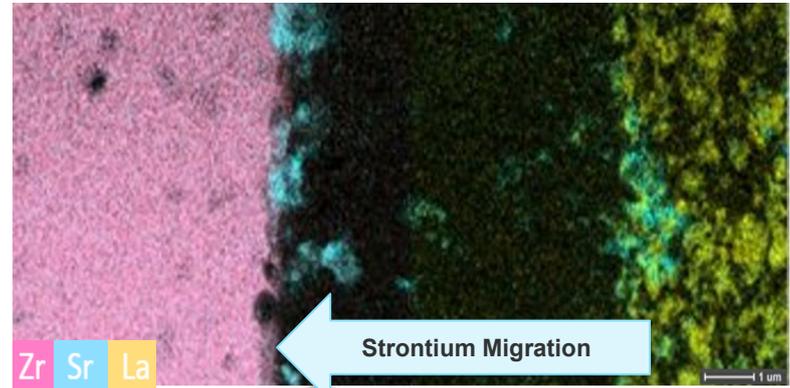
Zr, Sr, and La EDS map of the electrolyte, barrier layer, and oxygen electrode illustrating the migration of Sr

2D Nano-CT projections capturing the oxygen electrode and barrier layer interface in cells tested for a.) 50 and b.) 1k hours

Nano-CT images reveal interface densification occurring after extended cell operation, which may result in performance loss due to restricted mass and ionic transport
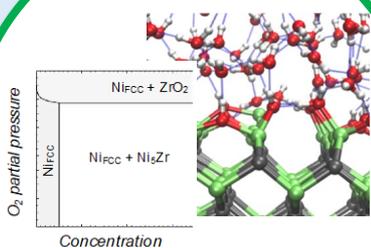
High Temperature Electrolysis (HTE)

Task 8: Multiscale Modeling
(more content in AMR Poster P196g)

H₂NEW
U.S. DEPARTMENT OF ENERGY

Multi-Scale Degradation Modeling- Approach

*Models suggest that not just **operating conditions**, but also **microstructural features** and **Ni loading** can impact the direction and magnitude of Ni redistribution*

Synthetic

Ni	YSZ	Pore
49.6%	30.0%	20.3%
44.5%	35.3%	20.2%
39.9%	40.0%	20.1%
34.5%	45.8%	19.7%
30.0%	50.1%	19.9%

PFIB Reconstructed

Ni	YSZ	Pore
39.4%	43.2%	17.4%
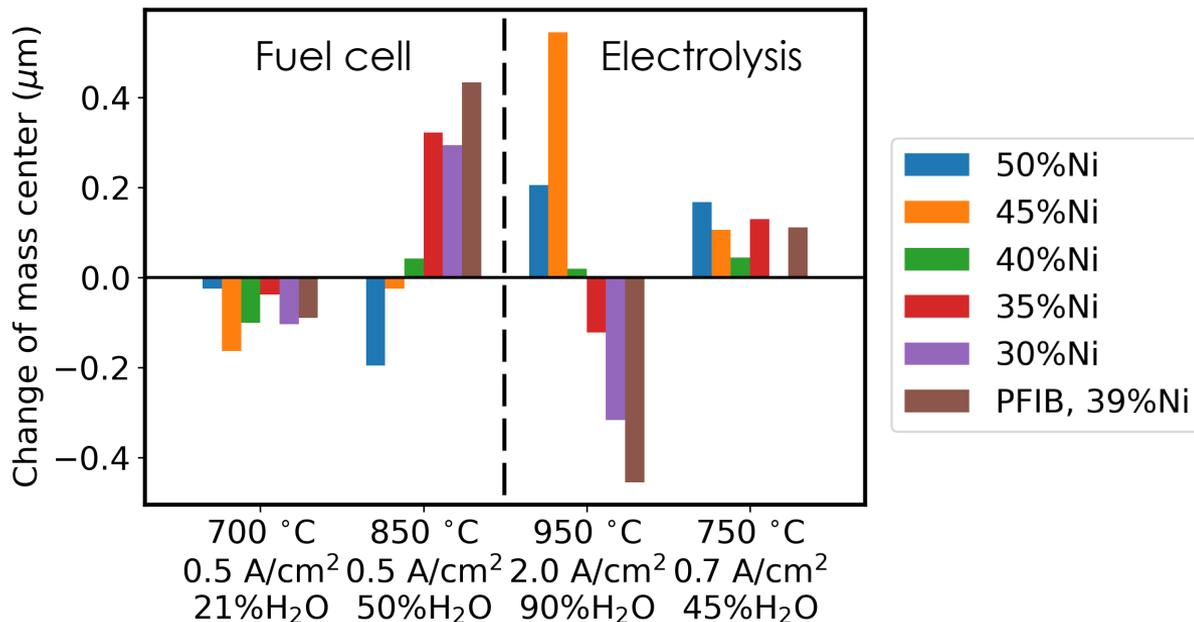
Accomplishment: Demonstrated multiscale framework for predicting Sr penetration into packed GDC as a possible failure mode

Porosity and loose particle packing create surface-dominated diffusion pathway for Sr and other cation impurities, with full permeation of GDC interlayer predicted as possible under operation
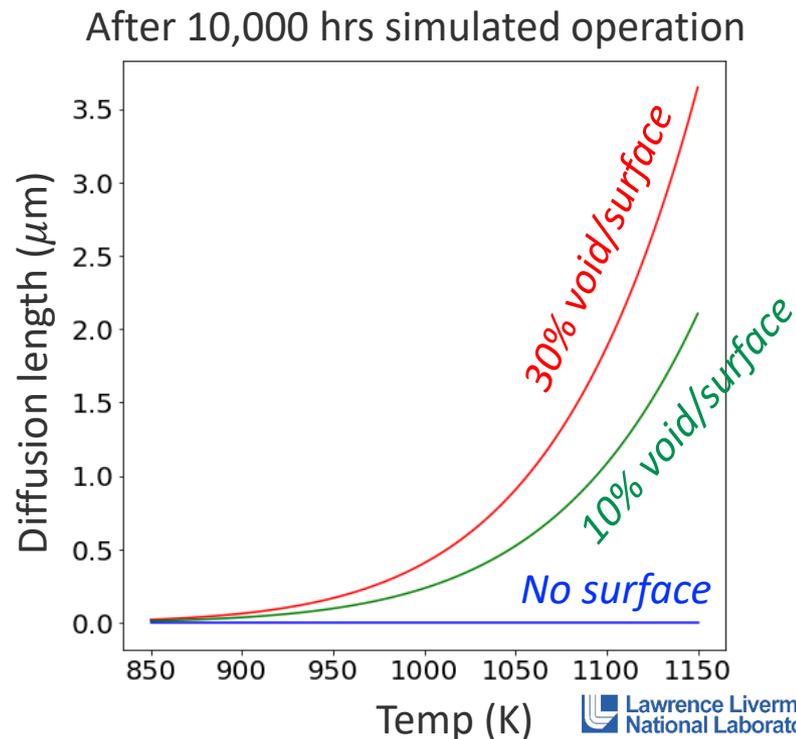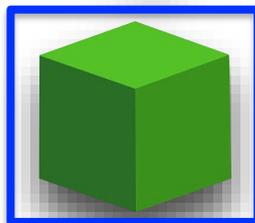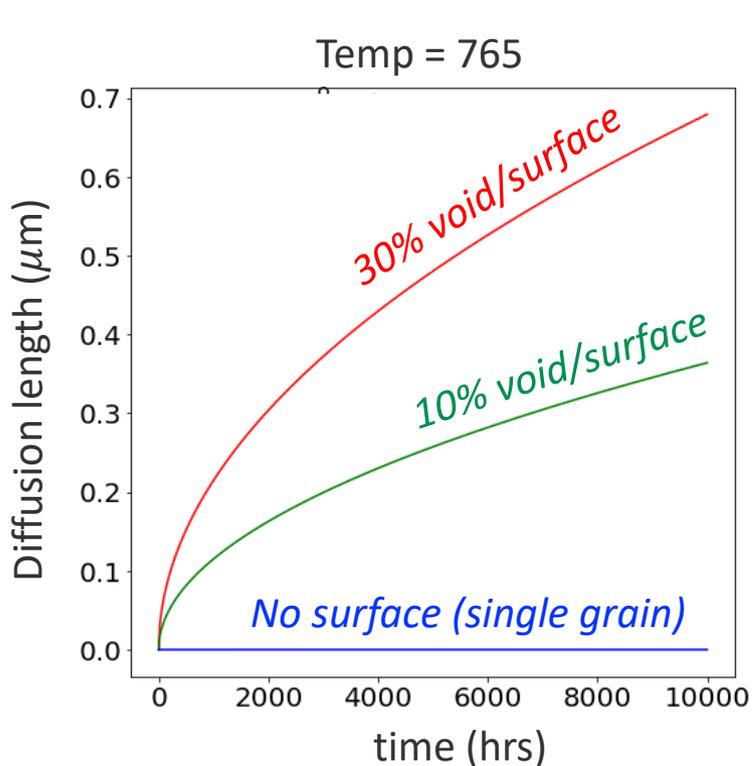
Ab initio calculations parameterize multiscale model and show that Sr diffusion is enhanced by local O vacancy concentration and presence of surfaces

Sr on GDC surface

Sr within GDC grain

Predicted diffusion of Sr in $Gd_xCe_{1-x}O_{2-0.5x}$

Diffusivity (cm^2/s)

T^{-1} (K^{-1})

$x = 0.1$
$x = 0$
Surface

$x = 0.1$
$x = 0$
Grain

Lawrence Livermore
National Laboratory
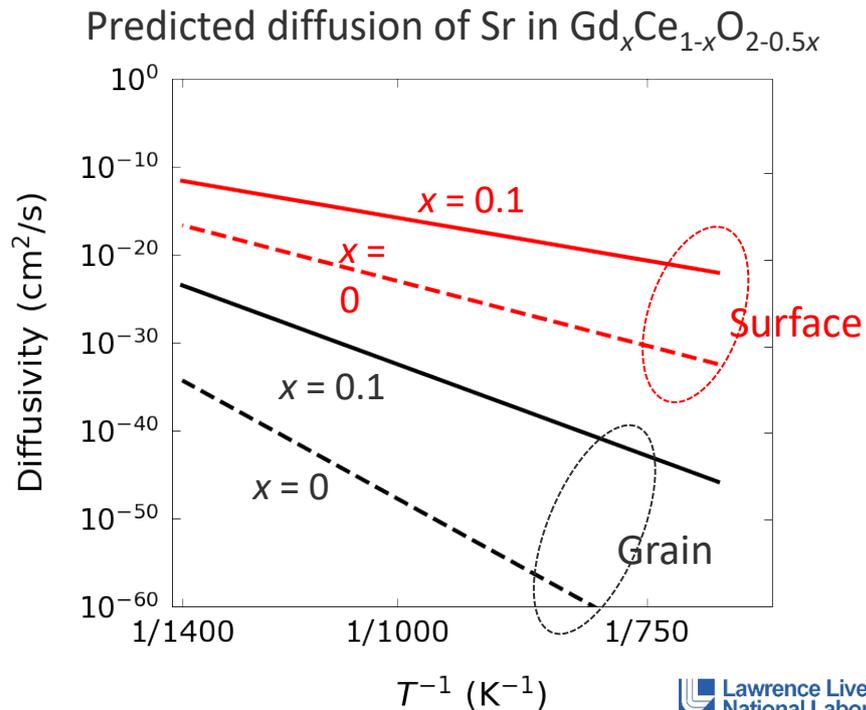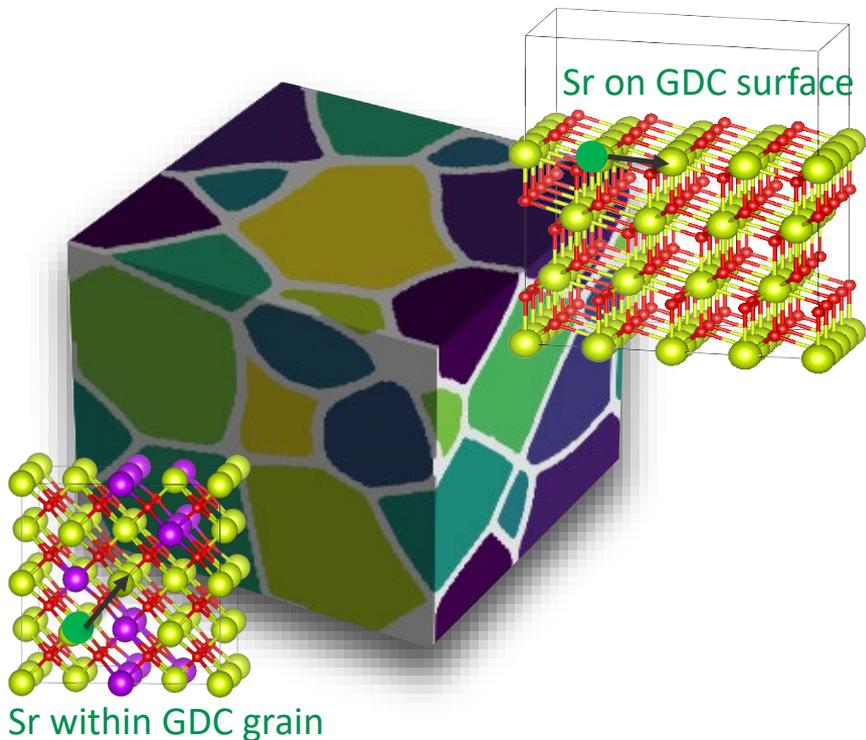
Responses to Previous Year Reviewers' Comments
(Project wasn't reviewed in FY 22, but FY 21 comments below)

- **Reviewer Comment:** The project is performed solely by national laboratories, so industry participation is largely missing.
- **Response:** We have done what we can to incorporate this through our Advisory Board and other engagement with industrial partners, but this is in the process of changing with release of HFTO FOA 2922.

- **Reviewer Comment:** Alkaline electrolysis is not addressed in the project, yet there have been substantial technology advances in recent years, and it is likely to capture a large market share in 2030 and beyond.
- **Response:** As can be seen in this presentation, Alkaline is now part of H2NEW and discussed in detail.

- **Reviewer Comment:** There is no mention of other emerging technologies, such as HTE proton-conducting technology or LTE anion exchange membrane technology.
- **Response:** This was by design and is beyond the scope of H2NEW for now and is covered in HydroGEN (2.0).

- **Reviewer Comment:** The project is focused on standard technologies and material sets. It would be great to see some investigation into promising alternatives that have the potential to leapfrog over the existing state of the art.
- **Response:** This is also changing as HFTO FOA 2922 addresses this area and there is also a Lab Call out supporting novel materials development that will feed into H2NEW activities.

Task 1 (Durability): Aging Studies; Mitigation Strategies; Ex-situ Characterization of MEAs/components/interfaces; Ex-situ Catalyst Durability; Ex-situ Membrane Durability; Accelerated Stress Test Development

Task 2 (Performance): Performance benchmarking, baselining, validation; Cell performance testing in support of electrode development; Ex-situ studies focused on performance factors; Cell level model development

Task 3 (Scale-up): MEA fabrication, Interface engineering (inks, electrodes, cell integration and interfaces); Components (porous transport layers, recombination layers)

Task 3c (Analysis): Performance, manufacturing, and system models; Durability factors; Energy system integration

Task 9 (Alkaline): Fundamental degradation mechanisms, AST development, Benchmarking, Baselines, Modeling, Scale-up

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

Task 5: Durability Testing and AST Development

i. SOEC materials and component degradation mechanisms are the result of multiple, coupled phenomena derived from operating conditions and a comprehensive and accurate understanding of the interplay of these phenomena remains to be established

ii. Larger planar cell test stand capacity is needed to fully understand cell degradation phenomena

Task 6: Task Integration and Protocol Validation

i. H2NEW is generating large volumes of data that require review, validation, and interpretation

Task 7: Advanced Characterization

i. In-operando testing is needed to reduce the number of test samples and to expedite AST outcomes

Task 8: Multiscale Modeling

i. Defining and modeling the mechanisms requires the combined talents, experience and capabilities of each of the Lab Consortium

ii. Degradation processes at the YSZ|GDC|LSCF-SDC interface are probably coupled in a non-linear fashion

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

Collaboration and Coordination

NREL Team Members: Shaun Alia, Carlos Baez-Cotto, Guido Bender, Sarah Blair, Ai-Lin Chan, Sunil Khandavalli, Chang Liu, Scott Mauger, Samantha Medina, Elliot Padgett, Makenzie Parimuha, Chance Parrish, Jason Pfeilsticker, Bryan Pivovar, Robin Rice, Meital Shviro, Abi Schmeiser, Michael Ulsh, Sam Ware, Jacob Wrubel, James Young, Jason Zack , David Ginley, Sarah Shulda

INL Team Members: Richard Boardman, Dong Ding, Micah Casteel, Lucun Wang, Wie Wu, Jeremy Hartwigsen, Josh Gomez, Daniel Wendt, Fred Steward, Nick Kane

LBNL Team Members: Grace Anderson, Claire Arthurs, Ashley Bird, Ethan Crumlin, Arthur Dizon, Elizabeth Greenberg, Rebecca Hamlyn, Ahmet Kusoglu, Grace Lau, Jason Keonhag Lee, Jiangjin Liu, Rangachary Mukundan, Xiong Peng, Michael Tucker, Adam Weber

PNNL Team Members: Olga Marina, Jamie Holladay, Chris Coyle, Kerry Meinhardt, Dan Edwards, Matt Olszta, Nathan Canfield, Lorraine Seymour, Nathanael Royer, Jie Bao, Brian Koeppel

ANL Team Members: Rajesh Ahluwalia, C. Firat Cetinbas, Luke Johnson, Nancy N. Kariuki, Samuel J. Kazmouz, A. Jeremy Kropf, Debbie Myers, Dennis Papadias, Jae Hyung Park, Jui-Kun (Michael) Peng, Xiaohua Wang, Di-Jia Liu

ORNL Team Members: David Arregui-Mena, Jefferey Baxter, Dave Cullen, Neus Domingo, Xiang Lyu, Harry Meyer, Shawn Reeves, Alexey Serov, Hanyu Wang, Haoran Yu, Michael Zachman

LANL Team Members: Tanvir Arman, Sergio Diaz-Abad, Kaustubh Khedekar, Siddharth Komini Babu, Kui Li, Jacob Spendelow, Mahlon Wilson, Abdurrahman Yilmaz

LLNL Team Members: Brandon Wood, Kyoung Kweon, Joel Berry, Penghao Xiao, Tim Hsu, Namhoon Kim

NETL Team Members: Harry Abernathy, Greg Hackett

NIST Affiliate Team Members: Daniel Hussey, David Jacobson, Jacob LaManna

SLAC: Nick Strange

University Collaborators: Jayson Foster, Svitlana Pylypenko (PI), Lonneke van Eijik, Max Shepherd, Genevieve Stelmacovic, Brian Gorman (CSM); Kara Ferner, Shawn Litster (PI), Fausto Pasmay (CMU); Devashish Kulkarni, Jack Todd Lang, John Stansberry, Cliff Wang, Iryna Zenyuk (PI) (UCI); Scott Barnett, Peter Voorhees (NU), Xiao-Dong Zhou (UL-L)

ASTWG Collaborators: Kathy Ayers (Nel Hydrogen), Nemanja Danilovic (Electric Hydrogen), Corky Mittelsteadt (Plug Power), Andrew Park (Chemours), Udit Shrivastava (Cummins), Andrew Smeltz (De Nora)

Other Partnerships and Collaborations: MIT, B. Khaykovich; FZ Jülich, Germany; Fraunhofer ISE, Freiburg, Germany; Paul Scherrer Institute, Aargau, Switzerland, IEA Annex 30 Working Group; Gen-IV International Forum for Hydrogen Production (Canada, France, Japan, England, United States)

Summary

- Significant science advances within H2NEW since inception
  - Establishment of capabilities (staff/facilities)
  - Execution of R&D scope
- Significant expansion in 2023 tied to Bipartisan Infrastructure Law (BIL) funding
  - Expansion of PEM and O-SOEC scope
  - Addition of LAWE as a R&D area
- HFTO FOA 2922 and Lab Call DE-LC-0000022 to leverage H2NEW assets and expand scope of efforts to date – novel materials development and supply chain considerations in particular.