H2NEW
Hydrogen from
Next-generation
Electrolyzers of Water
U.S. DEPARTMENT OF ENERGY

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

HFTO H_2 Production Lead: Dave Peterson
Director: Bryan Pivovar, National Renewable Energy Laboratory (NREL)
Deputy Director: Richard Boardman, Idaho National Laboratory (INL)

Date: 1/26/23
H2IQ Webinar

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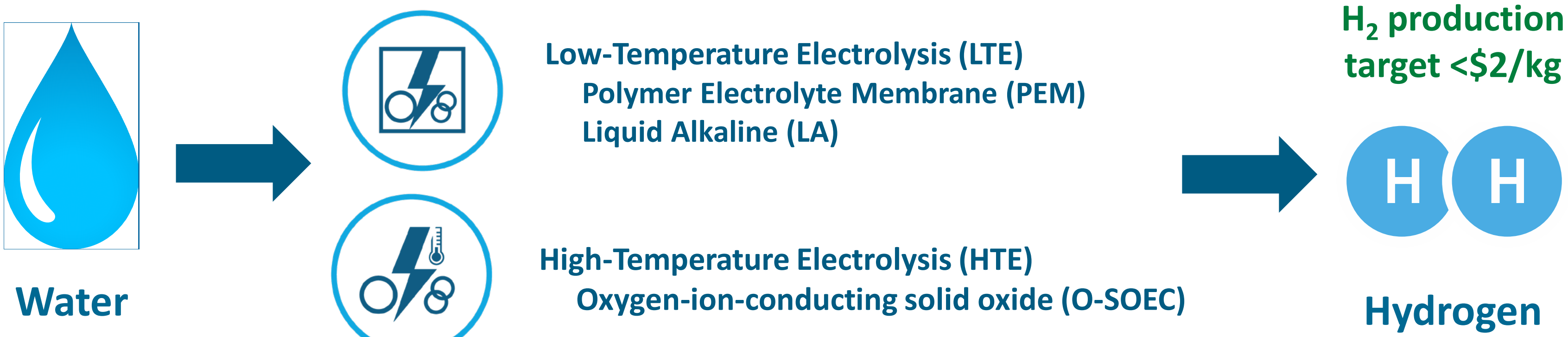
H2IQ Webinar Outline

- Overview of H2NEW – Rangachary Mukundan (LBNL)
- Low Temperature Electrolysis (LTE)
    - TEA/System Analysis – Bryan Pivovar (NREL)
    - Baselining/Benchmarking efforts – Debbie Myers (ANL)
    - Ir/Anode durability – Debbie Myers (ANL)
    - PTLs – Guido Bender (NREL)
    - Liquid Alkaline (Emerging) – Guido Bender (NREL)
- High Temperature Electrolysis (HTE) – Richard Boardman (INL)
    - HTE Technical Targets – Micah Casteel (INL)
    - Cell Fabrication and Accelerated Stress Testing – Olga Marina (PNNL)
    - Materials Degradation Modeling – Brandon Wood (LLNL)
    - Synchrotron SOEC characterization – Sarah Shulda (NREL)
- H2NEW website as community resource – Sarah Shulda (NREL)

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 2025 on way to H2 Shot target, \$1/kg by 2031).



Water

Low-Temperature Electrolysis (LTE)
- **Polymer Electrolyte Membrane (PEM)**
- **Liquid Alkaline (LA)**

High-Temperature Electrolysis (HTE)
- **Oxygen-ion-conducting solid oxide (O-SOEC)**

H_2 production target <\$2/kg

Hydrogen

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)**

AMR presentations

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

Consortium Team*

NREL NATIONAL RENEWABLE ENERGY LABORATORY
INL Idaho National Laboratory
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Pacific Northwest NATIONAL LABORATORY
Los Alamos NATIONAL LABORATORY
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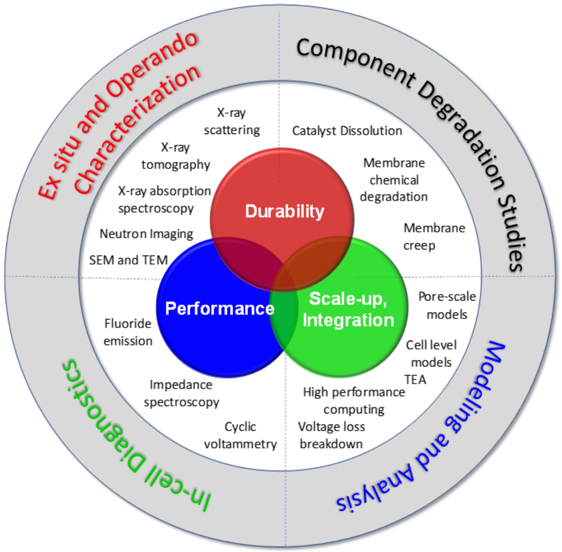
Lawrence Livermore National Laboratory

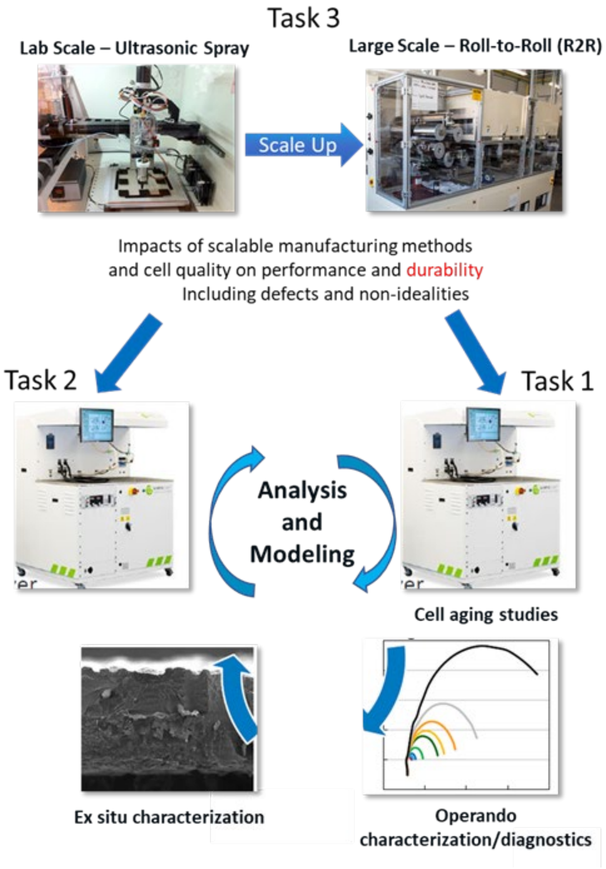
- NIST
- UC-Irvine
- Carnegie Mellon Univ
- Colorado School of Mines

* Expansion to include additional academic and industrial partners in anticipated in the near future through FOA projects

General Approach

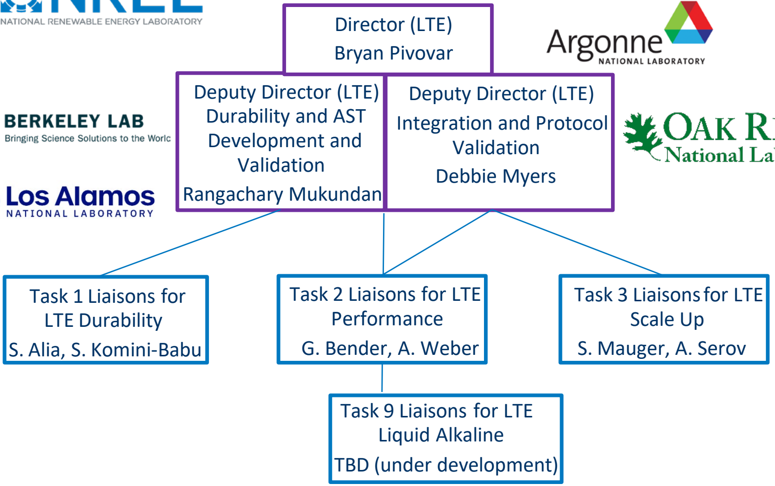


- **Durability (Task 1)**
  - Establish fundamental degradation mechanisms
  - Develop accelerated stress tests
  - Determine cost, performance, durability tradeoffs
  - Develop mitigation
  - https://www.hydrogen.energy.gov/pdfs/review22/p196a_myers_2022_p.pdf
- **Performance (Task 2)**
  - Benchmark performance
  - Novel diagnostic development and application
  - Cell level models and loss characterization
  - https://www.hydrogen.energy.gov/pdfs/review22/p196b_weber_2022_p.pdf
- **Scale-up (Task 3)**
  - Transition to mass manufacturing
  - Correlate processing with performance and durability
  - Guide efforts with systems and technoeconomic analysis (Task 3c, P196d)
  - https://www.hydrogen.energy.gov/pdfs/review22/p196c_ulsh_2022_p.pdf
  - https://www.hydrogen.energy.gov/pdfs/review22/p196d_ruth_2022_p.pdf



Impacts of scalable manufacturing methods and cell quality on performance and durability Including defects and non-idealities

Consortium Structure



Director (LTE)
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Deputy Director (LTE)
Durability and AST Development and Validation
Rangachary Mukundan

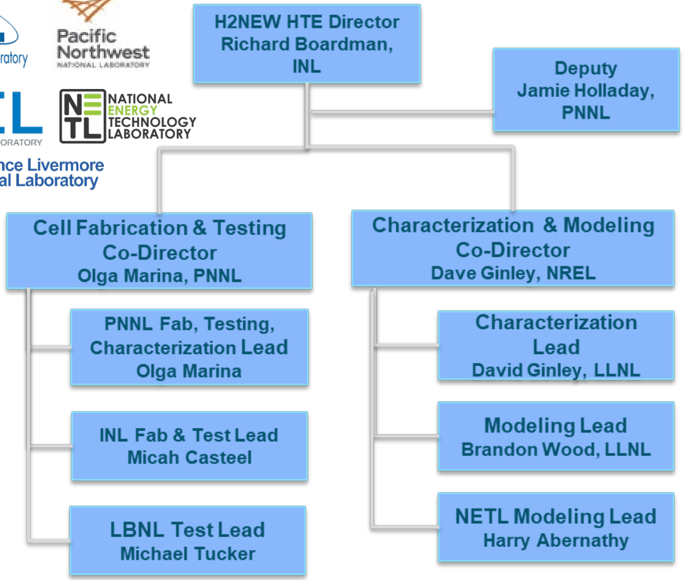
Deputy Director (LTE)
Integration and Protocol Validation
Debbie Myers

Task 1 Liaisons for LTE Durability
S. Alia, S. Komini-Babu

Task 2 Liaisons for LTE Performance
G. Bender, A. Weber

Task 3 Liaisons for LTE Scale Up
S. Mauger, A. Serov

Task 9 Liaisons for LTE Liquid Alkaline
TBD (under development)



H2NEW HTE Director
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Deputy
Jamie Holladay, PNNL

Cell Fabrication & Testing Co-Director
Olga Marina, PNNL

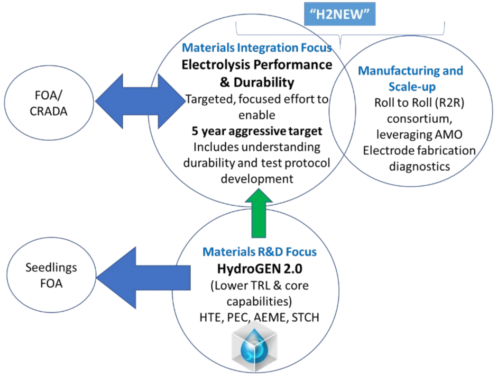
- PNNL Fab, Testing, Characterization Lead
  Olga Marina
- INL Fab & Test Lead
  Micah Casteel
- LBNL Test Lead
  Michael Tucker

Characterization & Modeling Co-Director
Dave Ginley, NREL

- Characterization Lead
  David Ginley, LLNL
- Modeling Lead
  Brandon Wood, LLNL
- NETL Modeling Lead
  Harry Abernathy

- 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



Leverage across other consortia:

HydroGEN 2.0 (HFTO)

R2R (AMO)

Million Mile Fuel Cell Truck (HFTO)

ElectroCat 2.0 (HFTO)

LTE Strategic 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)

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.

- HTE Stakeholder Advisory Board
  - **Scott Swartz**, Nexceris; **Greg Tao**, Chemtronergy; **Tony Leo**, Fuel Cell Energy; **Elango Elangovan** and **Joe Hartvigsen**, OxEon Energy; **John Pietras**, St. Gobain; **Bryan Blackburn**, Redox Power Systems; **Scott Barnett**, Northwestern; **Xiao-Dong Zhou**, University of Louisiana-Lafayette

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Select LTE Highlight Areas

- Highlighting capabilities, impact, and direction
  - Technoeconomic and Systems Analysis
  - Baselining efforts
  - Ir/Anode durability
  - Porous Transport Layers (PTLs)
  - Alkaline

H2NEW Activities: Low Temperature Electrolysis (LTE)

Techno-economic and Systems Analysis

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Focus on understanding of optimized operating and deployment strategies

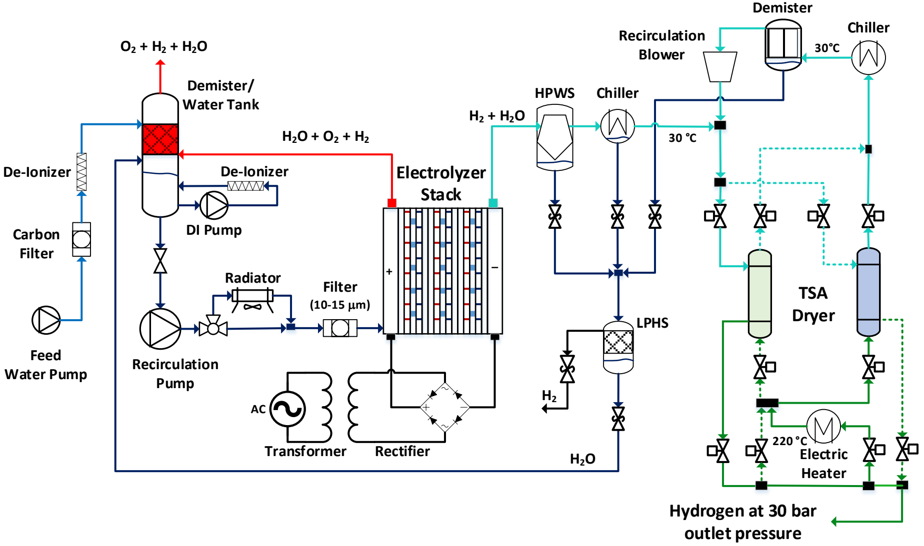
- Electrolyzers to date operate 24/7 at rated output
  - can’t chase cheap electrons or balance the energy system
  - over-engineered
- Predict/explore range of deployment options and assess impact on cost, performance, and durability
- Target is Hydrogen Levelized Cost and H_2 shot targets (\$1kg H_2 in 1 decade)
- Base cases include
  - traditional – 24/7 operation
  - grid integrated (highly variable)
  - direct coupled to solar and/or wind
- Has different impacts/capabilities depending on electrolyzer type
  - Polymer electrolyte membrane (PEM), liquid alkaline (LA), solid oxide (O-SOEC)

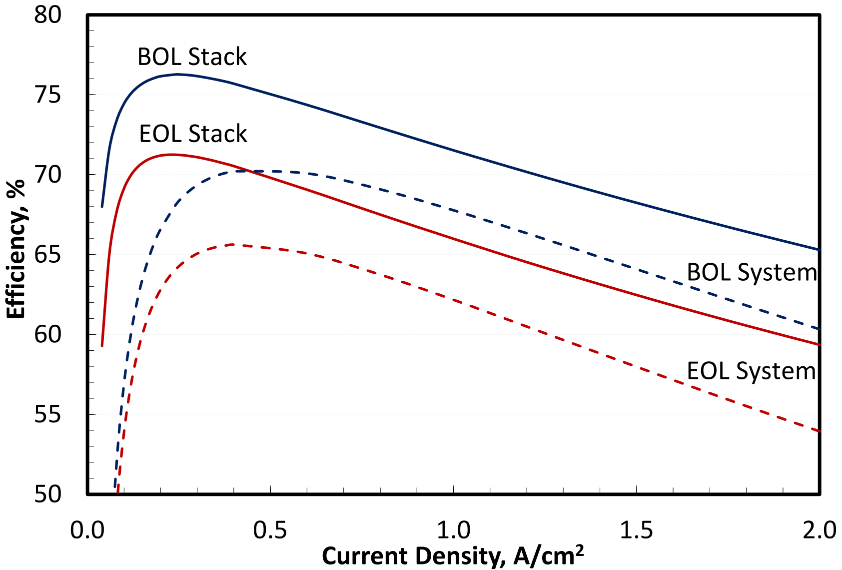
PEM Electrolysis Systems Analysis

PEM Electrolysis Systems Analysis

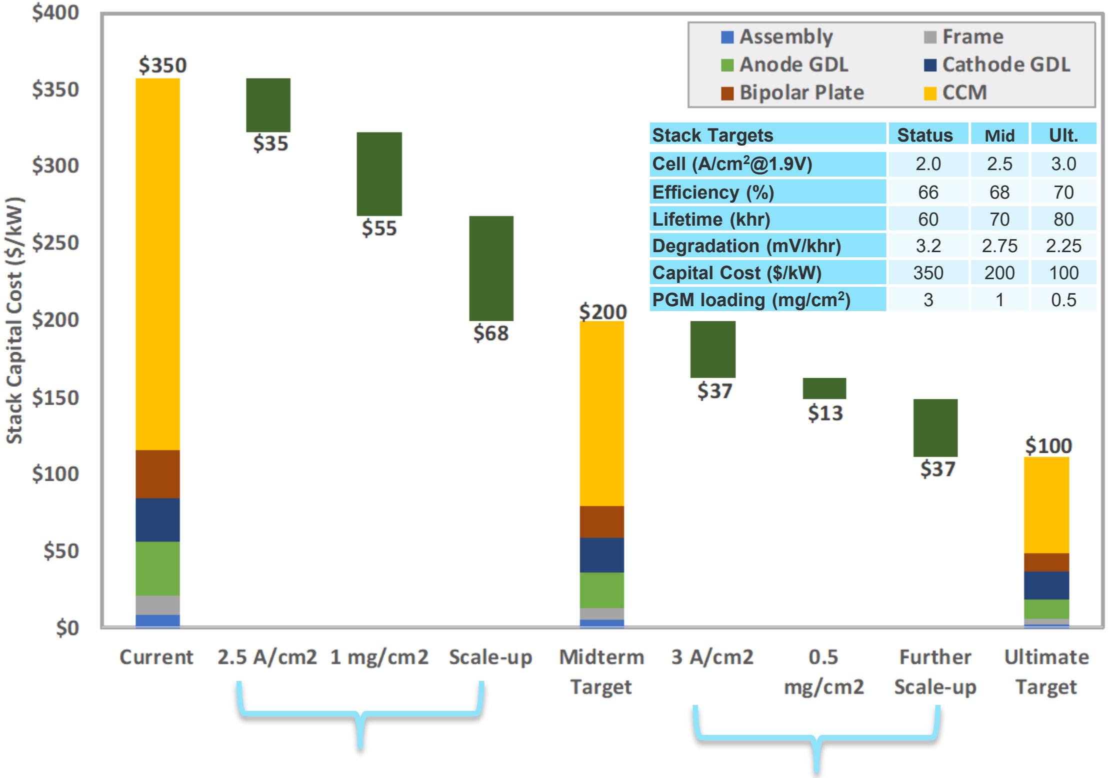
- Baseline system design allows for evaluation of cost and efficiency
- Can be modified and results flow into techno-economic analysis that results in levelized cost of hydrogen

	Efficiency (%)		Efficiency (kWh/kg-H_2)	
	BOL	EOL	BOL	EOL
Stack				
Rated Power Efficiency	65.3	59.3	51.1	56.2
Peak Efficiency	76.3	71.2	43.7	46.8
System				
Rated Power Efficiency	60.3	53.9	55.3	61.8
Peak Efficiency	70.2	65.6	47.5	50.8

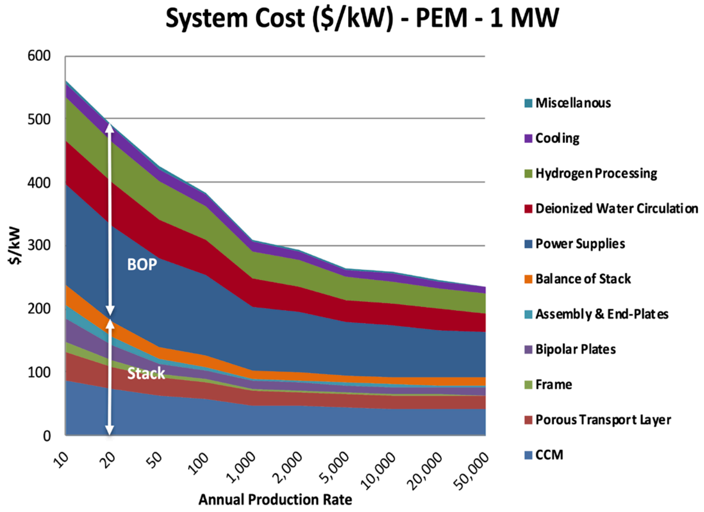




Stack Costs (PEM Centric to date)



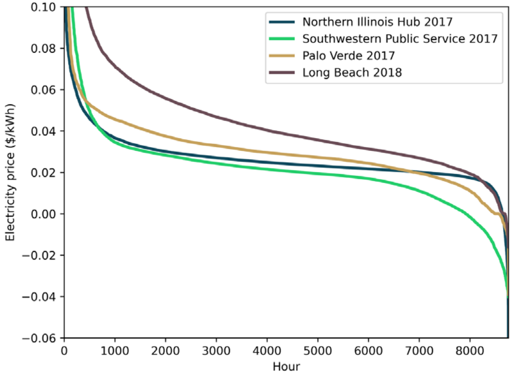
Stack Targets	Status	Mid	Ult.
Cell (A/cm^2@1.9V)	2.0	2.5	3.0
Efficiency (%)	66	68	70
Lifetime (khr)	60	70	80
Degradation (mV/khr)	3.2	2.75	2.25
Capital Cost ($/kW)	350	200	100
PGM loading (mg/cm^2)	3	1	0.5



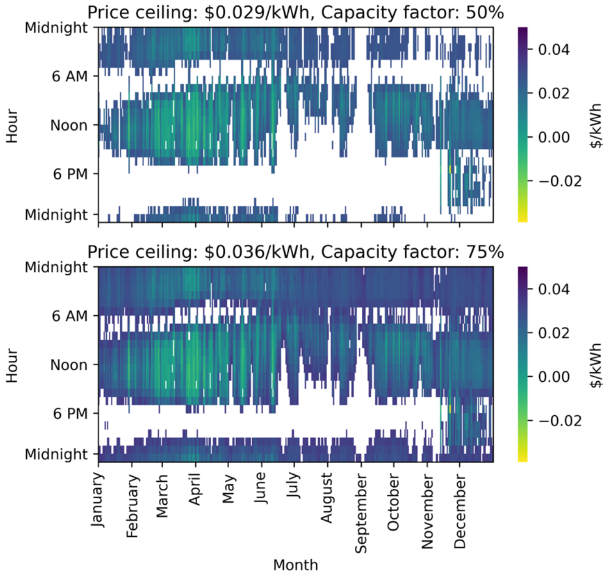
Modeling of stack costs show strongest levers are:

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

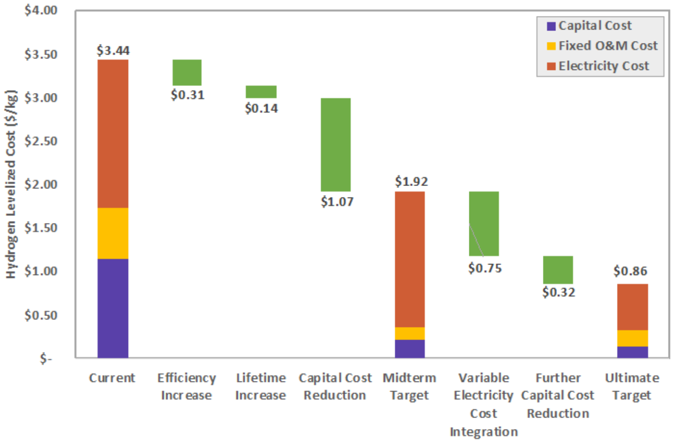
Electricity Market Impacts



- Past, current, and (projected) future wholesale electricity prices under investigation



- Locational marginal pricing taken into consideration
- Impact on operating strategies considered



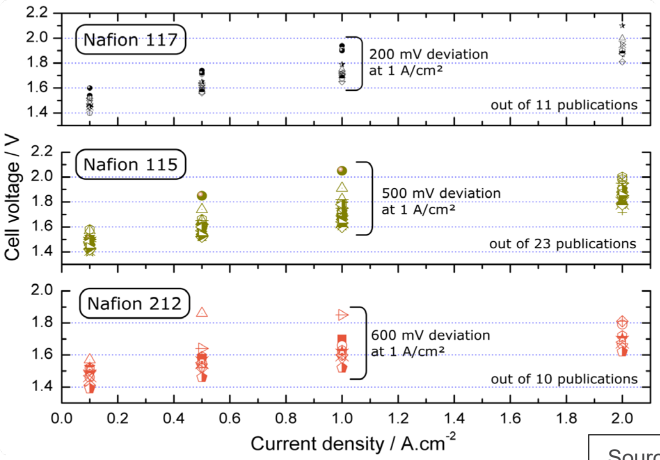
- Impact of electricity cost on hydrogen levelized costs are calculated
- Pathways to achieve lowest cost investigated

H2NEW Activities: Low Temperature Electrolysis (LTE)

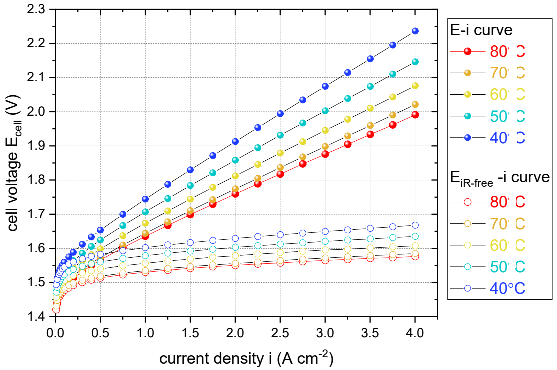
Baselining Efforts

Motivation and Approach of PEM Baselining and Benchmarking

- Future electrolyzer systems require a shift from static operation of overengineered systems to dynamic intermittent operation of cost sensitive systems
- Variations of literature results slows down research efforts, limits understanding of materials properties in the community and undermines trust between institutions
- Benchmarking instills trust within the community, between laboratories, in literature results. It promotes collaborations and accelerates progress
- Baselining of materials is essential to determine current state-of-the-art, understand material property/performance relationships and accelerate development of next-generation material sets
- Standardizing Voltage Loss Breakdown Analysis (VBA) to understand cell losses and identify focus areas for research and development



Source: Bender et al, IJHE 44 (2019) 9174-918



- H2New test example for VBA analysis harmonization effort
- FuGeMEA IV performance results at various temperatures

Benchmarking Performance with IEA Annex 30

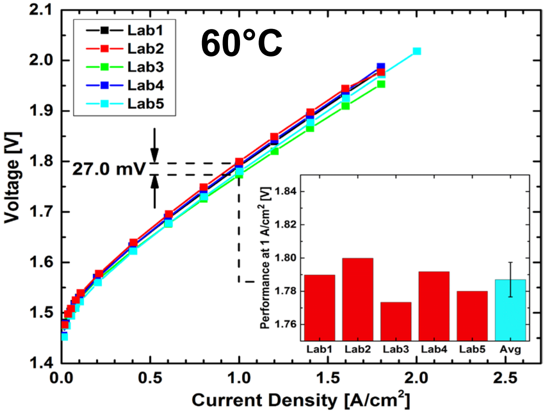
Phase 1

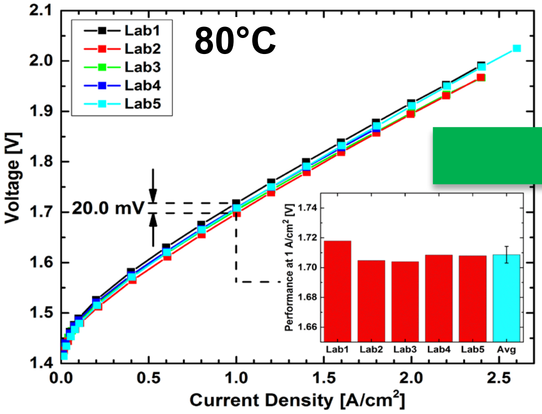
- Establish the basis for accurate data comparison across five laboratories
- Polarization curves with commercial MEA, defined hardware and operating conditions

Phase 2

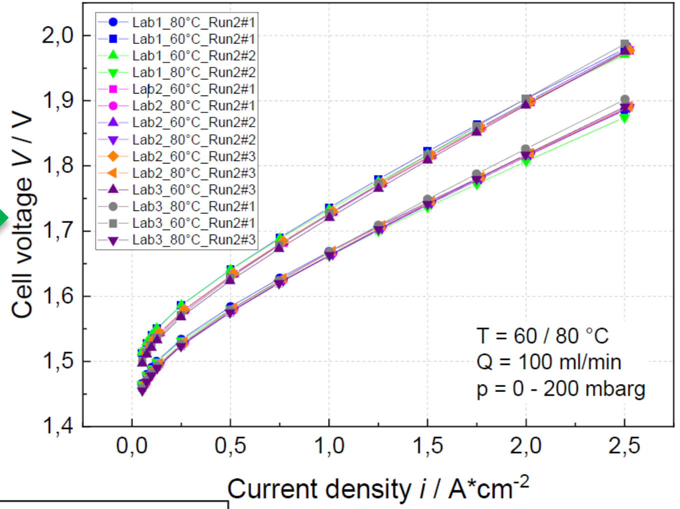
- Target stand. Dev. < 0.25 % of cell voltage
- Tighten test conditions
- Reference hardware & components
- Review & refine procedures

Current density / A*cm²	ΔUmax / mV (T = 60 °C)	ΔUmax / mV (T = 80 °C)
0.1	18	12
1	15 (27)	8 (20)
2	10	19





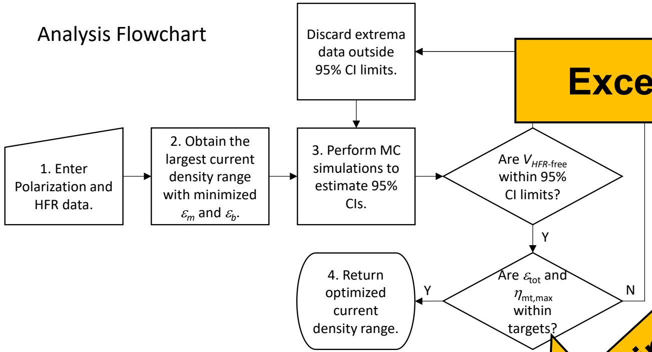
G. Bender et al, Int. J. of Hydrogen Energy, 44, 2019, 9174.



T. Lickert et al, in preparation

Harmonizing Voltage Breakdown Analysis

Flowchart



Analysis Flowchart

1. Enter Polarization and HFR data.

2. Obtain the largest current density range with minimized ε_m and ε_b.

3. Perform MC simulations to estimate 95% CIs.

Are $V_{HFR\text{-}free}$ within 95% CI limits?

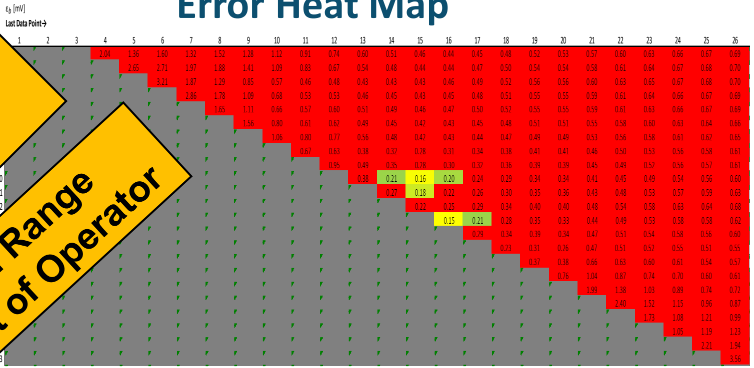
N: Discard extrema data outside 95% CI limits.

Y: Are ε_{tot} and $\eta_{mt,max}$ within targets?

N

Y: 4. Return optimized current density range.

Error Heat Map

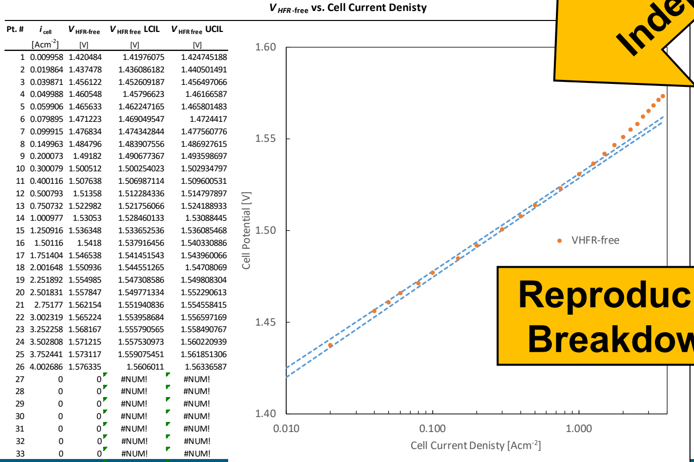


ε_b [mV] Last Data Point→	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26
				2.04	1.36	1.60	1.32	1.52	1.28	1.12	0.91	0.74	0.60	0.51	0.46	0.44	0.45	0.48	0.52	0.53	0.57	0.60	0.63	0.66	0.67	0.69
					2.65	2.71	1.97	1.88	1.41	1.09	0.83	0.67	0.54	0.48	0.44	0.44	0.47	0.50	0.54	0.54	0.58	0.61	0.64	0.67	0.68	0.70
						3.21	1.87	1.29	0.85	0.57	0.46	0.48	0.43	0.43	0.43	0.46	0.49	0.52	0.56	0.56	0.60	0.63	0.65	0.67	0.68	0.70
							2.86	1.78	1.09	0.68	0.53	0.53	0.46	0.45	0.43	0.45	0.48	0.51	0.55	0.55	0.59	0.61	0.64	0.66	0.67	0.69
								1.65	1.11	0.66	0.57	0.60	0.51	0.49	0.46	0.47	0.50	0.52	0.55	0.55	0.59	0.61	0.63	0.66	0.67	0.69
									1.56	0.80	0.61	0.62	0.49	0.45	0.42	0.43	0.45	0.48	0.51	0.51	0.55	0.58	0.60	0.63	0.64	0.66
										1.06	0.80	0.77	0.56	0.48	0.42	0.43	0.44	0.47	0.49	0.49	0.53	0.56	0.58	0.61	0.62	0.65
											0.67	0.63	0.38	0.32	0.28	0.31	0.34	0.38	0.41	0.41	0.46	0.50	0.53	0.56	0.58	0.61
												0.95	0.49	0.35	0.28	0.30	0.32	0.36	0.39	0.39	0.45	0.49	0.52	0.56	0.57	0.61
10													0.38	0.21	0.16	0.20	0.24	0.29	0.34	0.34	0.41	0.45	0.49	0.54	0.56	0.60
11														0.27	0.18	0.22	0.26	0.30	0.35	0.36	0.43	0.48	0.53	0.57	0.59	0.63
12															0.22	0.25	0.29	0.34	0.40	0.40	0.48	0.54	0.58	0.63	0.64	0.68
																0.15	0.21	0.28	0.35	0.33	0.44	0.49	0.53	0.58	0.58	0.62
																	0.29	0.34	0.39	0.34	0.47	0.51	0.54	0.58	0.56	0.60
																		0.23	0.31	0.26	0.47	0.51	0.52	0.55	0.51	0.55
																			0.37	0.38	0.66	0.63	0.60	0.61	0.54	0.57
																				0.76	1.04	0.87	0.74	0.70	0.60	0.61
																					1.99	1.38	1.03	0.89	0.74	0.72
																						2.40	1.52	1.15	0.96	0.87
																							1.73	1.08	1.21	0.99
																								1.05	1.19	1.23
																									2.21	1.94
23																										3.56

Excel Tool

Linear Tafel Range Independent of Operator

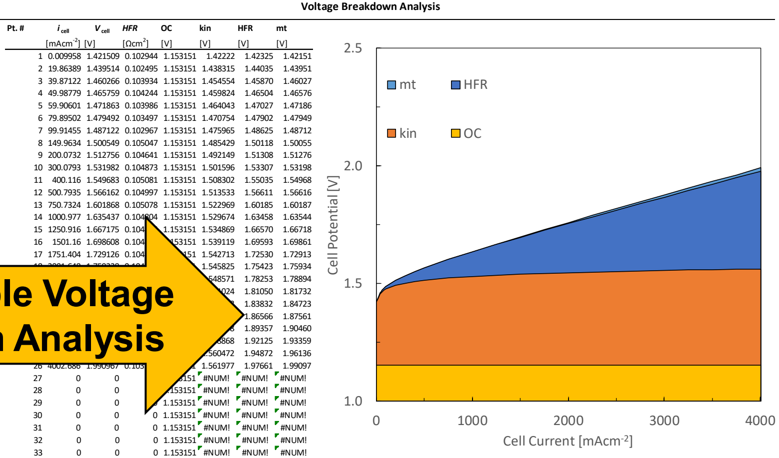
95% Confidence Intervals



$V_{HFR\text{-}free}$ vs. Cell Current Denisty

Pt. #	i_{cell} [Acm^{-2}]	$V_{HFR\text{-}free}$ [V]	$V_{HFR\ free}$ LCIL [V]	$V_{HFR\ free}$ UCIL [V]
1	0.009958	1.420484	1.41976075	1.424745188
2	0.019864	1.437478	1.436086182	1.440501491
3	0.039871	1.456122	1.452609187	1.456497066
4	0.049988	1.460548	1.45796623	1.46166587
5	0.059906	1.465633	1.462247165	1.465801483
6	0.079895	1.471223	1.469049547	1.4724417
7	0.099915	1.476834	1.474342844	1.477560776
8	0.149963	1.484796	1.483907556	1.486927615
9	0.200073	1.49182	1.490677367	1.493598697
10	0.300079	1.500512	1.500254023	1.502934797
11	0.400116	1.507638	1.506987114	1.509600531
12	0.500793	1.51358	1.512284336	1.514797897
13	0.750732	1.522982	1.521756066	1.524188933
14	1.000977	1.53053	1.528460133	1.53088445
15	1.250916	1.536348	1.533652536	1.536085468
16	1.50116	1.5418	1.537916456	1.540330886
17	1.751404	1.546538	1.541451543	1.543960066
18	2.001648	1.550936	1.544551265	1.54708069
19	2.251892	1.554985	1.547308586	1.549808304
20	2.501831	1.557847	1.549771334	1.552290613
21	2.75177	1.562154	1.551940836	1.554558415
22	3.002319	1.565224	1.553958684	1.556597169
23	3.252258	1.568167	1.555790565	1.558490767
24	3.502808	1.571215	1.557530973	1.560220939
25	3.752441	1.573117	1.559075451	1.561851306
26	4.002686	1.576335	1.5606011	1.56336587
27	0	0	#NUM!	#NUM!
28	0	0	#NUM!	#NUM!
29	0	0	#NUM!	#NUM!
30	0	0	#NUM!	#NUM!
31	0	0	#NUM!	#NUM!
32	0	0	#NUM!	#NUM!
33	0	0	#NUM!	#NUM!

Voltage Breakdown



Voltage Breakdown Analysis

Pt. #	i_{cell} [mAcm^{-2}]	V_{cell} [V]	*HFR* [Ωcm^2]	OC [V]	kin [V]	HFR [V]	mt [V]
1	0.009958	1.421509	0.102944	1.153151	1.42222	1.42325	1.42151
2	19.86389	1.439514	0.102495	1.153151	1.438315	1.44035	1.43951
3	39.87122	1.460266	0.103934	1.153151	1.454554	1.45870	1.46027
4	49.98779	1.465759	0.104244	1.153151	1.459824	1.46504	1.46576
5	59.90601	1.471863	0.103986	1.153151	1.464043	1.47027	1.47186
6	79.89502	1.479492	0.103497	1.153151	1.470754	1.47902	1.47949
7	99.91455	1.487122	0.102967	1.153151	1.475965	1.48625	1.48712
8	149.9634	1.500549	0.105047	1.153151	1.485429	1.50118	1.50055
9	200.0732	1.512756	0.104641	1.153151	1.492149	1.51308	1.51276
10	300.0793	1.531982	0.104873	1.153151	1.501596	1.53307	1.53198
11	400.116	1.549683	0.105081	1.153151	1.508302	1.55035	1.54968
12	500.7935	1.566162	0.104997	1.153151	1.513533	1.56611	1.56616
13	750.7324	1.601868	0.105078	1.153151	1.522969	1.60185	1.60187
14	1000.977	1.635437	0.104804	1.153151	1.529674	1.63458	1.63544
15	1250.916	1.667175	0.104	1.153151	1.534869	1.66570	1.66718
16	1501.16	1.698608	0.104	153151	1.539119	1.69593	1.69861
17	1751.404	1.729126	0.104	151	1.542713	1.72530	1.72913
					1.545825	1.75423	1.75934
					548571	1.78253	1.78894
					024	1.81050	1.81732
						1.83832	1.84723
						1.86566	1.87561
						1.89357	1.90460
					868	1.92125	1.93359
					1.560472	1.94872	1.96136
26	4002.686	1.990967	0.103		1.561977	1.97661	1.99097
27	0	0		3151	#NUM!	#NUM!	#NUM!
28	0	0		153151	#NUM!	#NUM!	#NUM!
29	0	0		1.153151	#NUM!	#NUM!	#NUM!
30	0	0	0	1.153151	#NUM!	#NUM!	#NUM!
31	0	0	0	1.153151	#NUM!	#NUM!	#NUM!
32	0	0	0	1.153151	#NUM!	#NUM!	#NUM!
33	0	0	0	1.153151	#NUM!	#NUM!	#NUM!

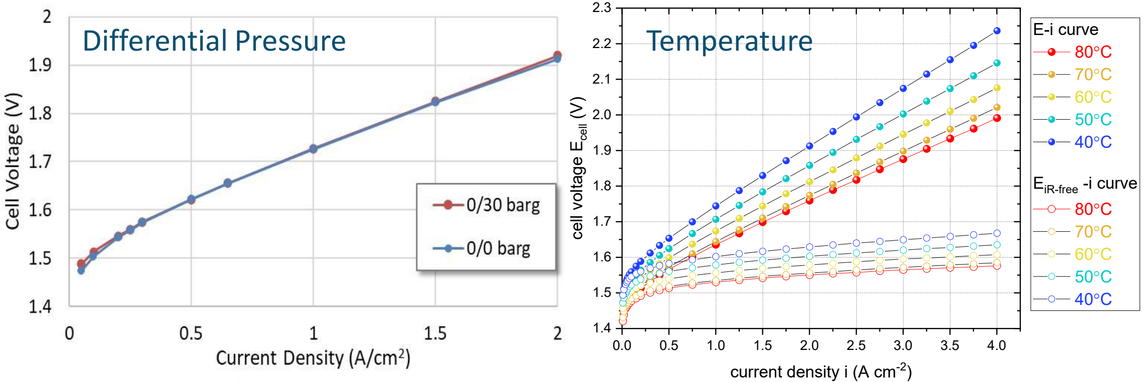
Reproducible Voltage Breakdown Analysis

- Algorithm in Excel:
  - Transparent
  - Portable
  - Easy to use
  - Easy to modify
- Copy paste process
- Highly reproducible results
- Will be open source and available to public
- Instruction video in making

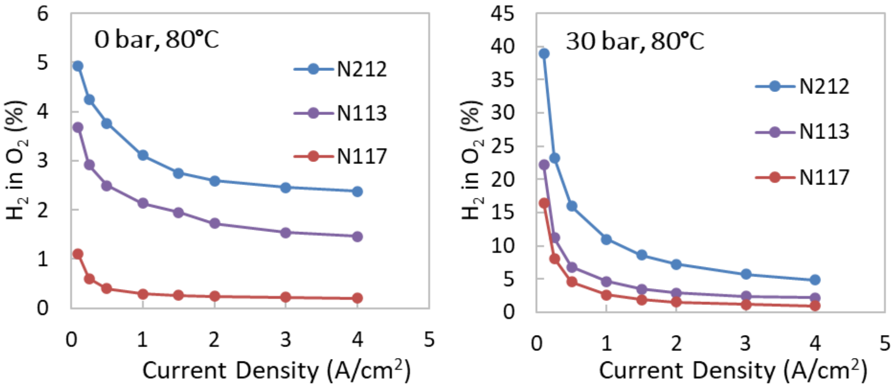
A. Dizon et al, in preparation

Baselining at industrially relevant conditions

Performance at various conditions



In-operando diagnostics



- FuGeMEA baseline material set: 0.4 mg IrOx, 0.1 mg Pt/C, N115, Pt-coated Ti-PTL, GDL
- High pressure hardware development
- Evaluating VI-performance and H2Xover performance of MEA systems
- Industrially relevant conditions and material sets

⇒ Determine current state-of-the-art materials sets & performances

⇒ Understand
  - Material property performance relationships
  - Interfaces
  - Cell processes

J. Wrubel et al., Int. J. of Hydrogen Energy, 47, 2022, 28244.

H2NEW Activities: Low Temperature Electrolysis (LTE)

Ir/Anode Durability

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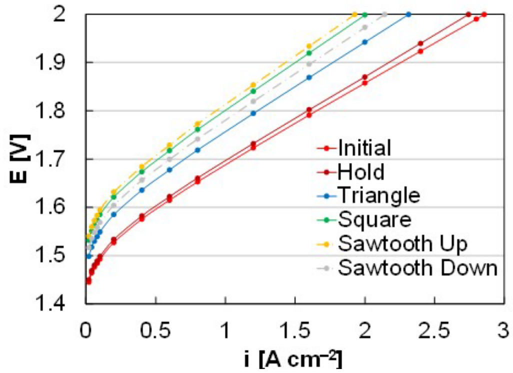
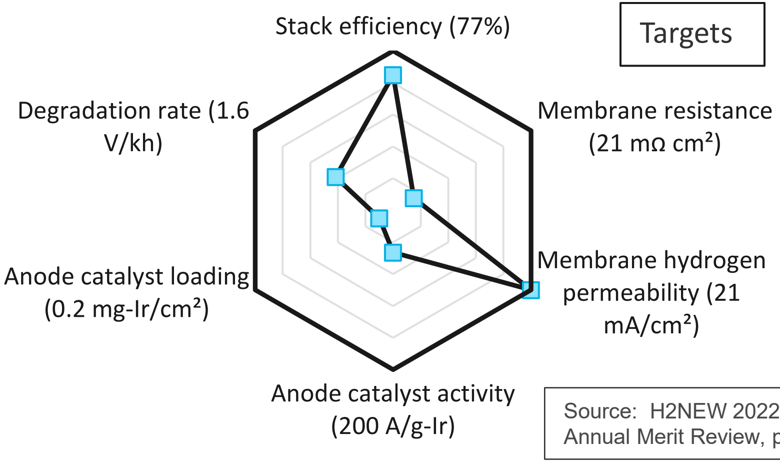
Fundamentals of Degradation/Mitigation approaches

- Little is understood about degradation in electrolyzers, particularly under dynamic conditions and cost-thrifted systems
- Systems to date have been “overengineered” and run continuously (mitigated stress)
- Target lifetime is ~10 years, accelerated stress tests needed but aren’t in place due to lack of fundamental understanding
- Combination of experimental data (in-situ, ex-situ, operando) and computational studies critical
- Need cost-performance-durability tradeoff information to feed into analysis efforts



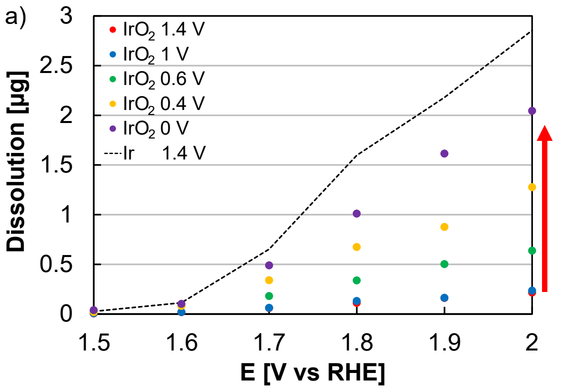


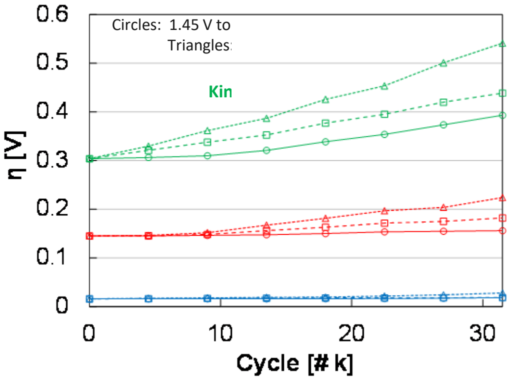
Source: H2NEW 2022 DOE Annual Merit Review, p. 196d

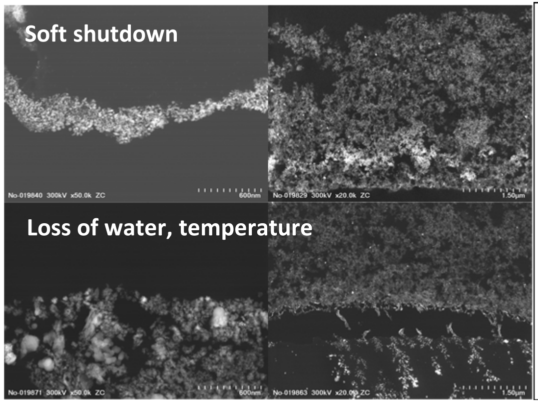
Durability: Accelerated Stress Test - Start-Stop

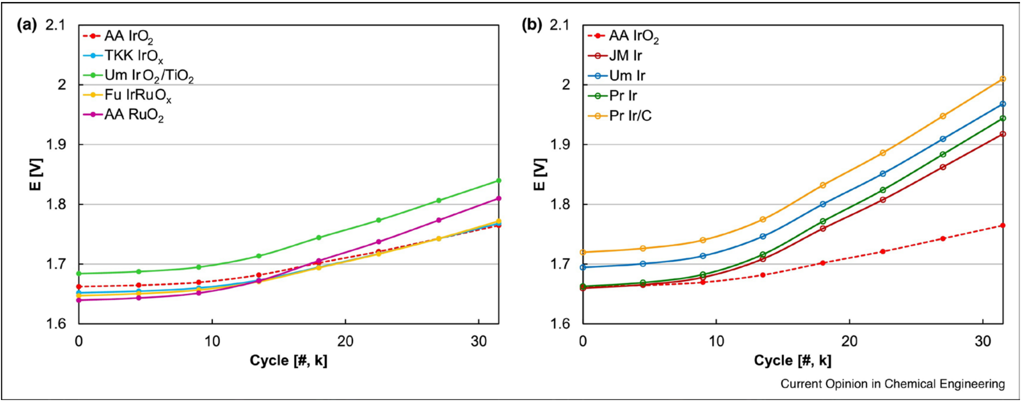
- MEAs: Nafion 117 (to mitigate crossover concerns)

  0.1 mg_M cm^{-2} anode catalyst loading
- Start-stop: Voltage control 0 to 2 V triangle (vs. intermittent: 1.45 to 2 V triangle)
- Summary of findings:
  - ✓ Higher performance losses for AST cycle through catalyst redox (0 to 2 V): major changes in particle size, not final oxidation state
  - ✓ Performance losses correlate with fraction of Ir in metallic state in catalyst used
  - ✓ Loss mechanism: thinning/increased PTL site-access, clear agglomeration, increased interfacial tearing

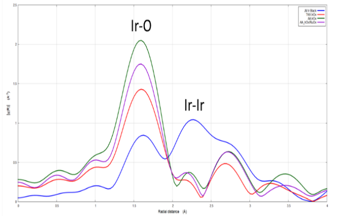


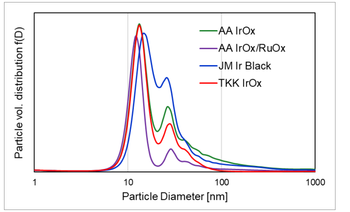






Current Opinion in Chemical Engineering

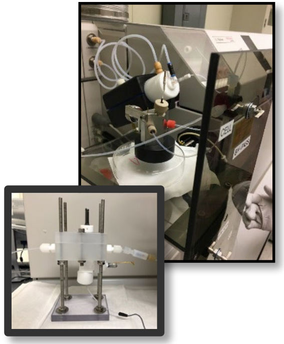


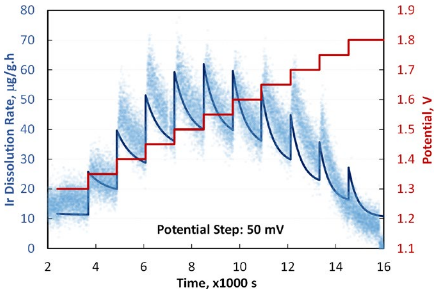


S.M. Alia, *Current Opinion in Chemical Engineering*, **2021**, 33, 100703.

Durability: Degradation studies of IrO_2 anode catalyst

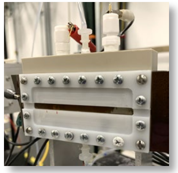
On-line Analysis of Catalyst Degradation Products (ICP-MS)

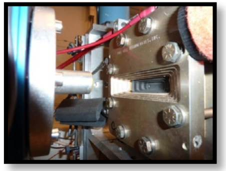


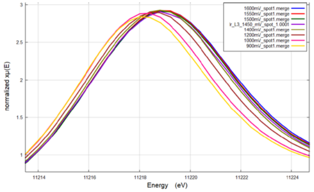


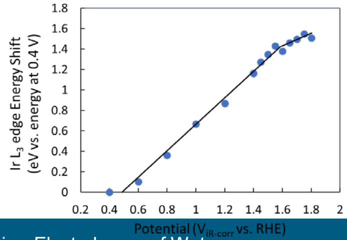
Points – data
Lines – model

In situ X-ray Absorption Spectroscopy









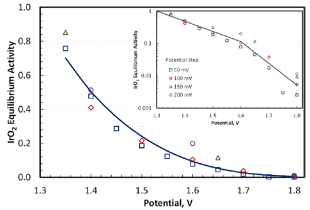
Modeling of Thermodynamics and Kinetics of Oxidation and Dissolution Reactions

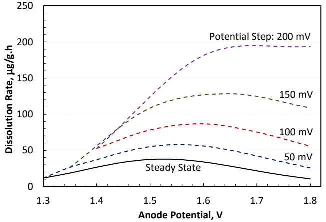
2-Species Dissolution Model

$IrO_2 + H_2O = IrO_2OH + H^+ + e^-$ (formation 1)
$IrO_2 + 2H_2O = IrO_4^{2-} + 4H^+ + 2e^-$ (diss. 1)
$IrO_2OH + H_2O = IrO_4^{2-} + 3H^+ + e^-$ (diss. 2)

$$IrO_2 + H_2O = IrO_2OH + H^+ + e^-$$

$$\dot{r}_1^{f} = k_1^f(a_1)(a_1 - a_1^{eq})e^{\left(\frac{\alpha_1^f F}{RT}\left(E - E_{0,1}^f\right)\right)} = k_1^{f\prime}(a_1)(a_1 - a_1^{eq})$$





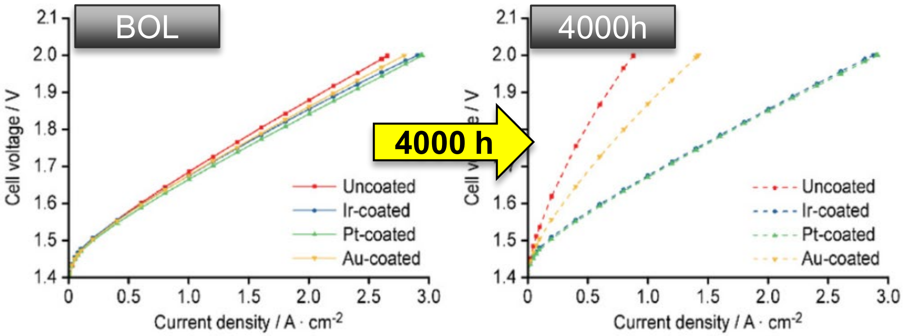
- Ir dissolution data modeled with dissolution of two species: IrO_2 and IrO_2OH, with the latter having slower dissolution kinetics
- Under steady-state conditions, catalyst is least stable at potentials between 1.5 and 1.55 V
- In situ X-ray data show appearance of higher oxidation state IrO_x species at 1.6 V – corresponding with suppression of dissolution

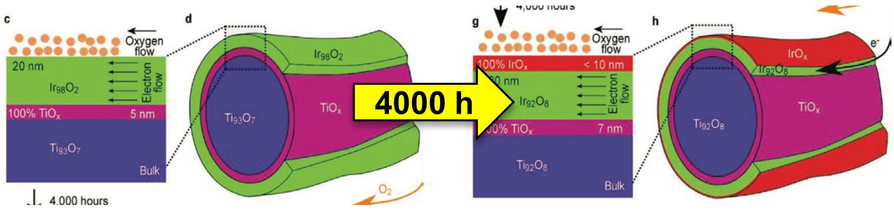
H2NEW Activities: Low Temperature Electrolysis (LTE)

Porous Transport Layers (PTLs)

Cell Component Characterization, Optimization & Integration

- Porous Transport Layers (PTL) are critical components for enabling:
    - High efficiency
    - Thin membranes
    - Low catalyst layer loadings
    - Differential pressure operation
    - Long term operation
- PTL and electrode layer trade off specific functionalities based on properties
- PTL property selection and integration into the cell are key to optimize performance and lifetime
- Routine and advanced characterization capabilities including operando techniques used to fully understand and optimize PTL functionalities





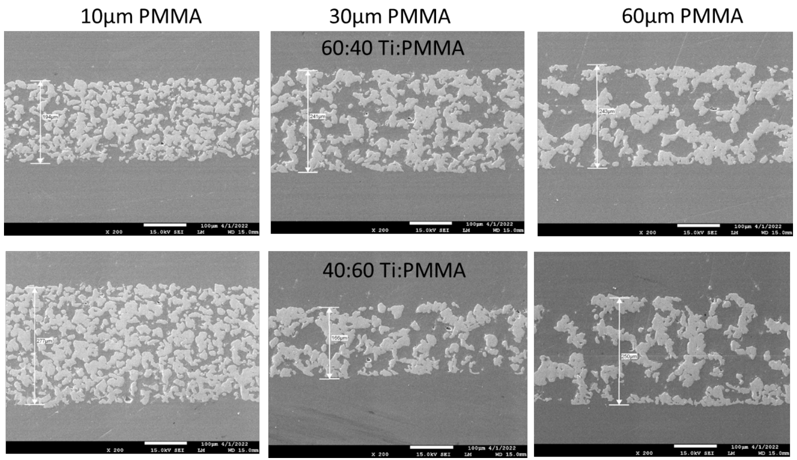
Source: Liu et al, Adv. Energy Mater. 2021, 11, 2002926

Ti PTL Pore Structure Optimization

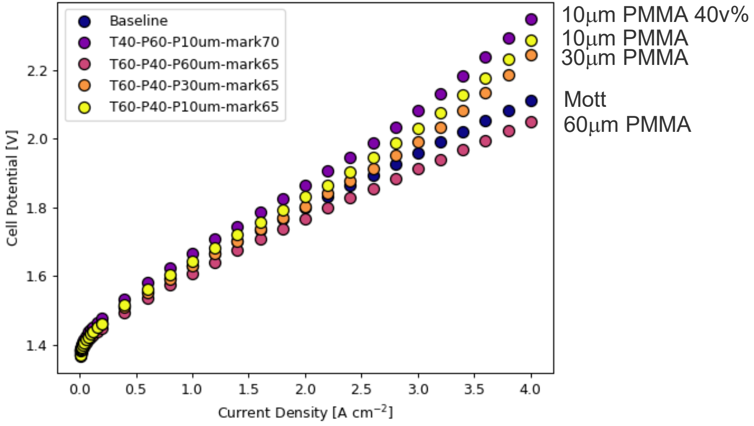
- Produced and tested PTLs with range of pore former size and loading
- Conducted ex-situ and in-situ characterization including VBA
- Result: 60 v% Ti – 40v% 60μm pore former outperforms baseline commercial PTL

80°C
N117 membrane
Anode: Tkk IrO_2 (0.4 mg/cm^2)
Cathode: Tkk10V50E Pt/C (0.1 mg/cm^2)
PTL thickness: 250 μm / gasket 250 μm
GDL: Toray 120 / gasket 250 μm

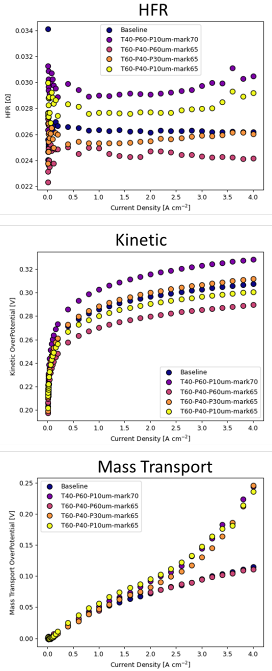
Tunable pore size and structure



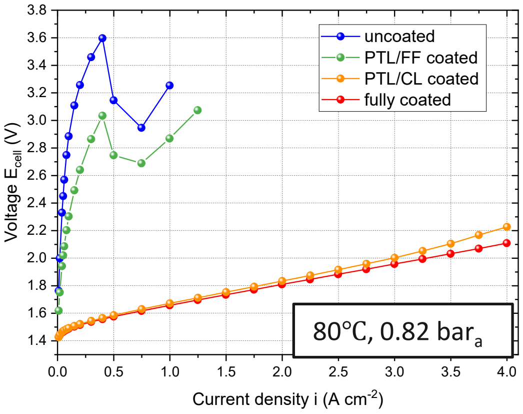
Cell Performance

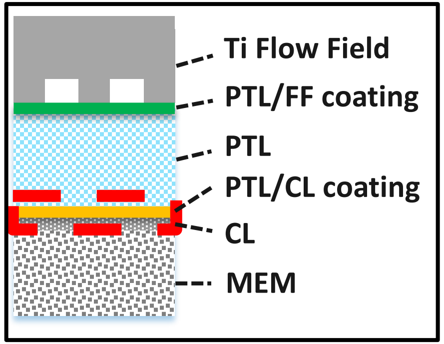


VBA Analysis

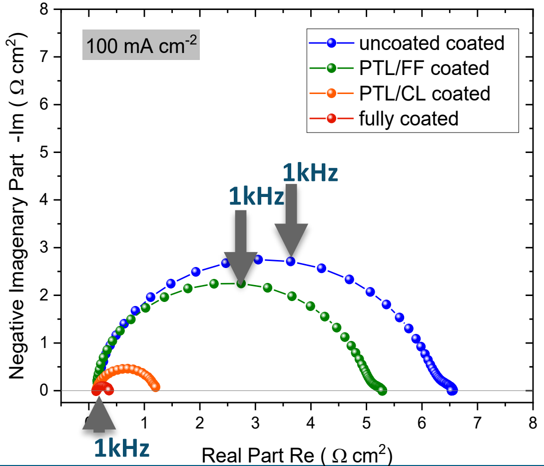


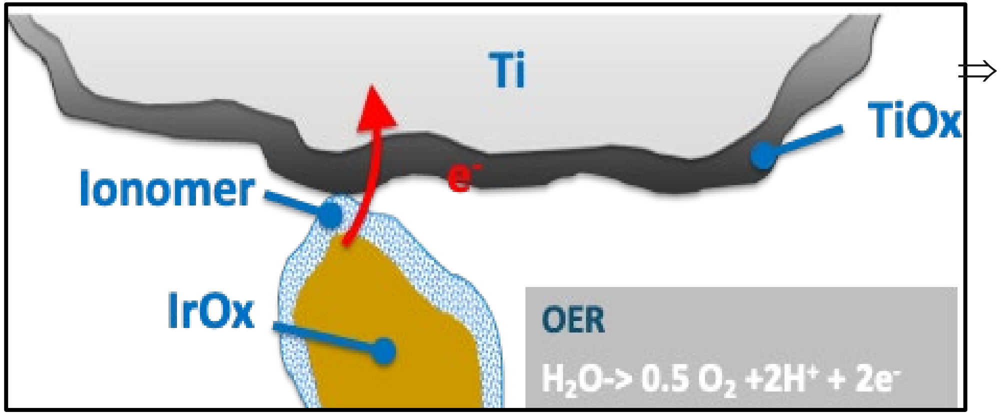
In-depth Study of PTL / Anode Interface





- Systematic study on the effect of PTL coatings for MEAs with low loading (FuGeMEA)
- PGM coating at the anode PTL/CL interface governs performance
- HFR data up to 300kHz indicate resistance is not the cause
- TiOx may act as a semiconductor and seems to be limiting the electron transfer

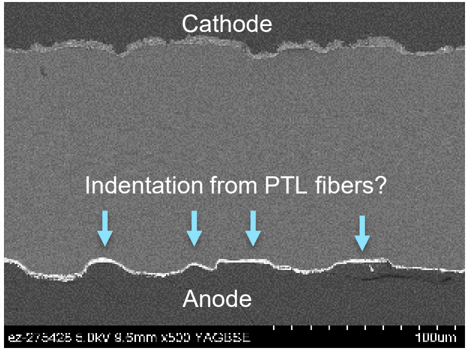


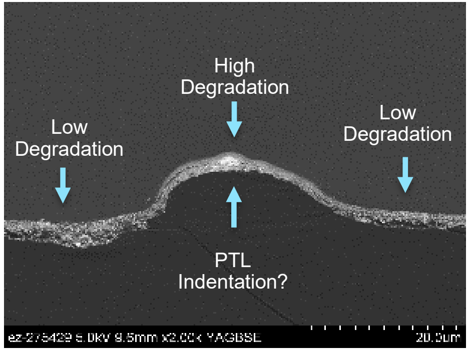


⇒ Pt interlayer creates Pt/TiOx junction

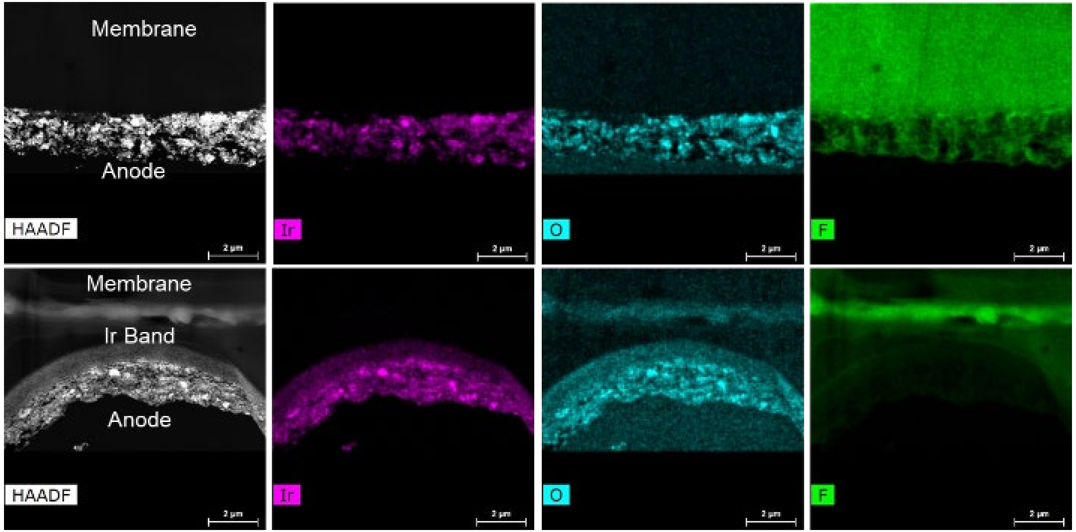
- Schottky diode metal/n-type ?
- Lower ohmic resistance

Tracking Inhomogeneous Degradation with Electron Microscopy





- Optical images show indentations in anode electrode from PTL fibers
- Similar indentations visible in cross-sectional SEM images correlate with degree of degradation



Low Degradation Regions:

- Limited Ir dissolution
- Similar electrode thickness and density to beginning-of-test MEA

High Degradation Regions:

- Band of dissolved Ir in membrane
- Denser electrode structure
- Curved electrode suggests direct contact with PTL

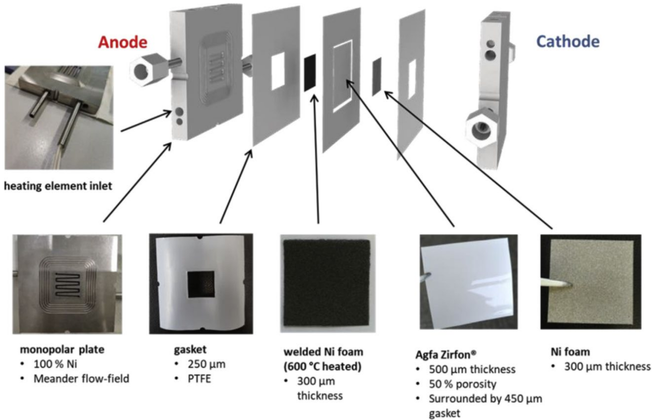
H2NEW Activities: Low Temperature Electrolysis (LTE)

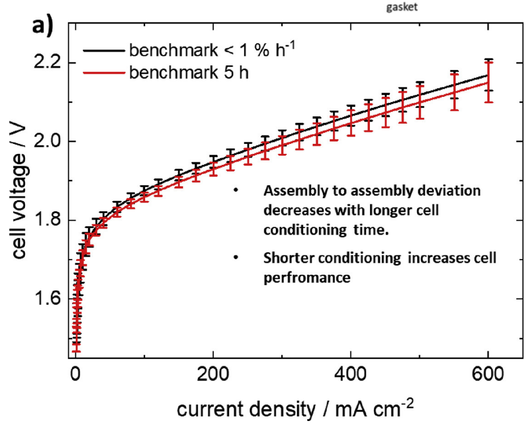
Liquid Alkaline

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)





- Assembly to assembly deviation decreases with longer cell conditioning time.
- Shorter conditioning increases cell perfromance

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

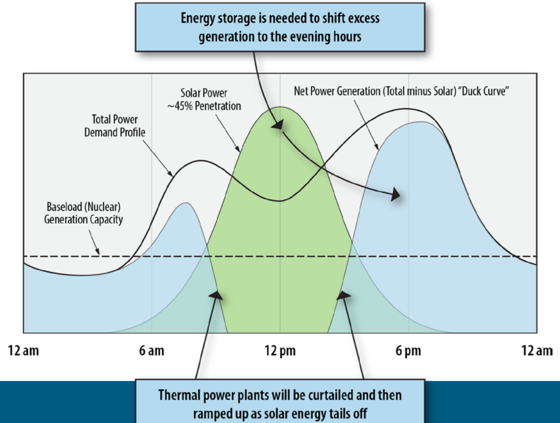
H2NEW Activities: High Temperature Electrolysis (HTE)

HTE focus on achieving high production efficiency for long-periods

- H2NEW Focus is on oxygen ion ($O^{=}$) electrolyte conducting SOEC (O-SOEC)
- O-SOEC development to date has overcome many challenges
  - Delamination of electrode/electrolyte layers
  - Materials coatings to prevent contamination and deactivation of catalysts
  - Lowered operating temperatures to reduce materials degradation

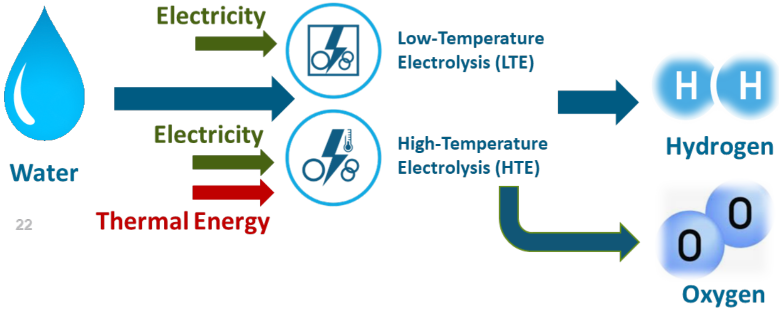
H2NEW applies accelerated stress testing of standard O-SOEC materials with deep characterization and multi-scale physics modeling to elucidate and predict microstructure evolution. This in turn will help optimize cell performance, cell geometry, and cell longevity

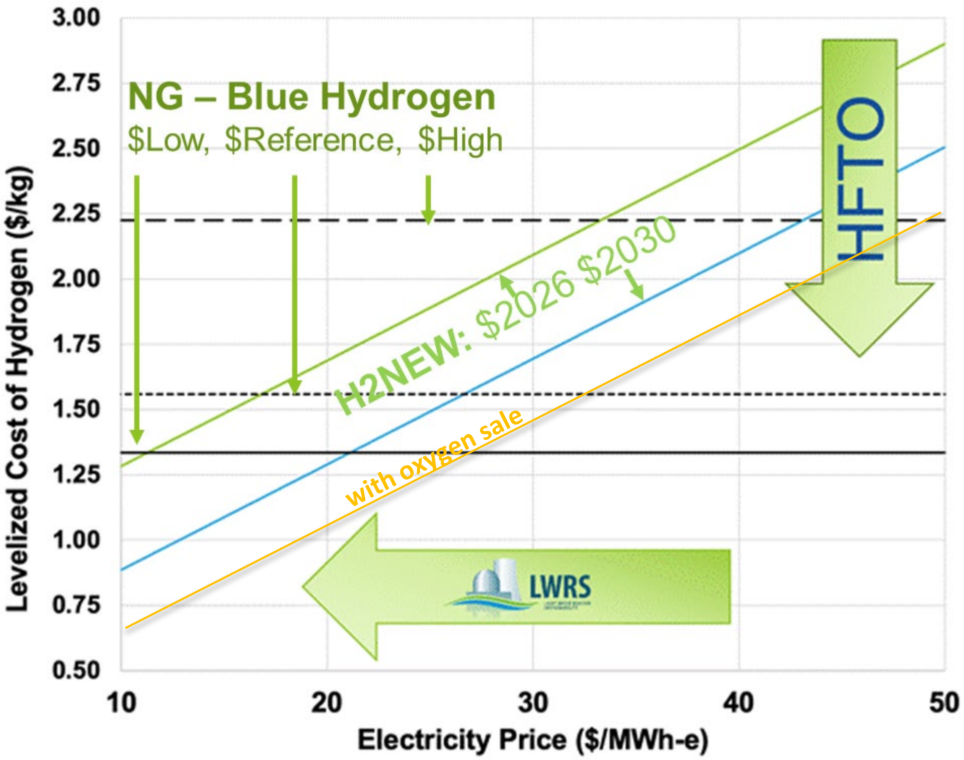
- SOEC hydrogen plants will generally be deployed near thermal power generation stations or embedded with industrial processes


Energy storage is needed to shift excess generation to the evening hours

Thermal power plants will be curtailed and then ramped up as solar energy tails off

HTE Approach to Earthshot Goal ($1/kg-H2 in 2030)





Select HTE Highlight Areas

- Highlighting capabilities, impact, and direction
  - HTE Technical Targets
  - Cell Fabrication and Accelerated Stress Testing
  - Materials Degradation Modeling
  - Synchrotron SOEC Characterization

  - Task 5 Durability and AST Development https://www.hydrogen.energy.gov/pdfs/review22/p196e_marina_2022_p.pdf
  - Task 6 Characterization https://www.hydrogen.energy.gov/pdfs/review22/p196f_ginley_2022_p.pdf
  - Task 8 Modeling https://www.hydrogen.energy.gov/pdfs/review22/p196g_wood_2022_p.pdf

H2NEW Activities: High Temperature Electrolysis (HTE)

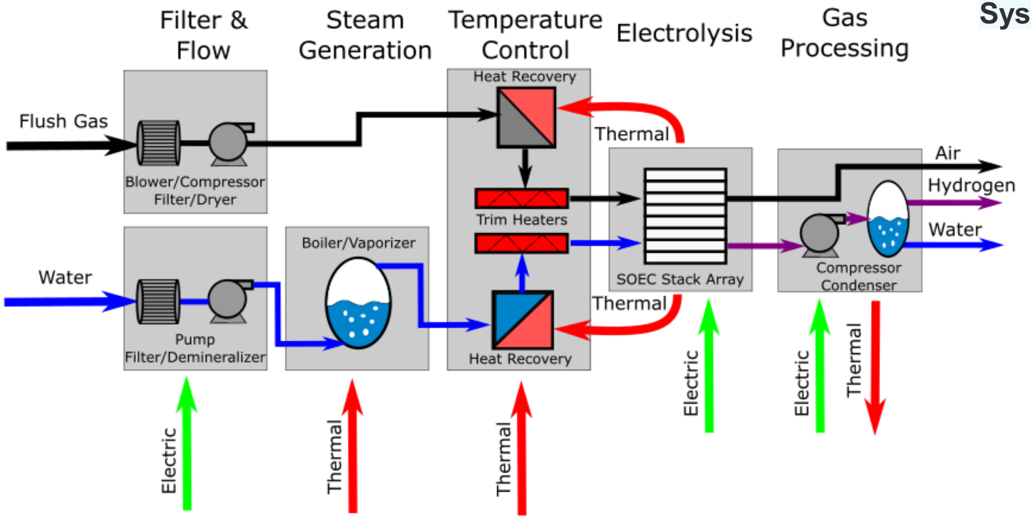
HTE Technical Targets

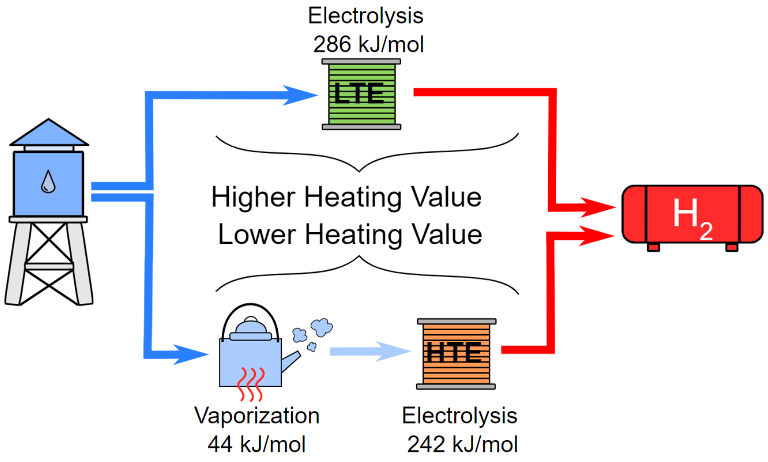
Technical Performance Targets

SOEC Electrolysis Systems Analysis

- Baseline system design allows for evaluation of cost and efficiency
- Results flow into techno-economic analysis that results in levelized cost of hydrogen

	2022 Status	Ultimate Target
Stack Efficiency	34 kWh/kg	34 kWh/kg
Current Density	0.6 A/cm2	2 A/cm2
Degradation	6.4 mv/kHr	1.5 mV/khr
Stack Lifetime	20,000 Hr	80,000 Hr
System Electrical Efficiency	38 kWh/kg	35 kWh/kg
System Total Efficiency	47 kWh/kg	42 kWh/kg





H2NEW Activities: High Temperature Electrolysis (HTE)

Cell Fabrication and Accelerated Stress Testing

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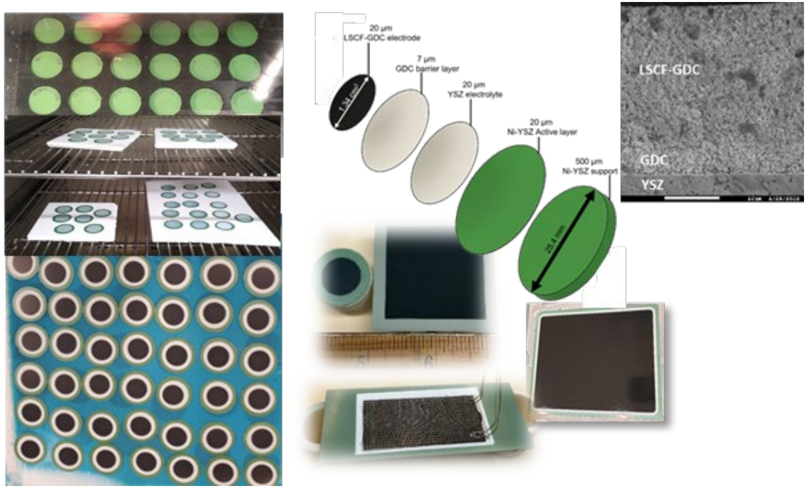
SOEC Cell Fabrication



- Identified representative state-of-the-art cell designs, materials, and fabrication techniques used by industry
- Developed a batch fabrication process to minimize the variance between the separate cells
- Initiated the development of QA/QC procedures
- Made cells available to all national labs for testing, performance validation, and characterization

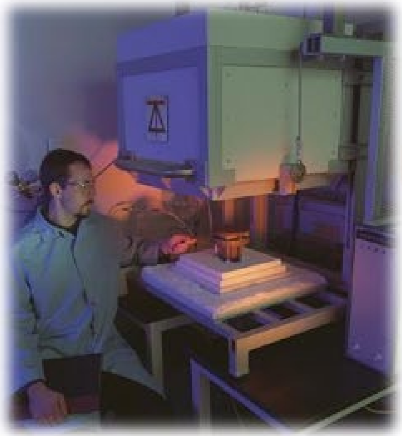
Testing of Multiple Cell Formats, from Button Cells to Stack Size Planar Cells

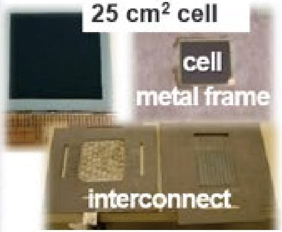
High throughput button cell testing

active area is 1-5 cm^2

- Materials screening
- I-V and EIS
- pH_2O=1-99%
- Impurities

Larger size planar cell testing



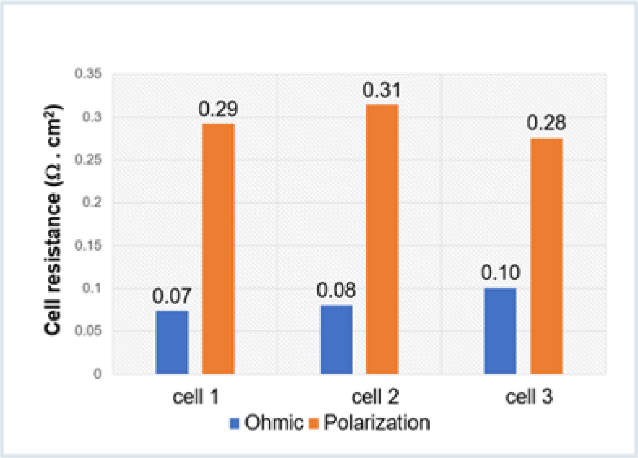


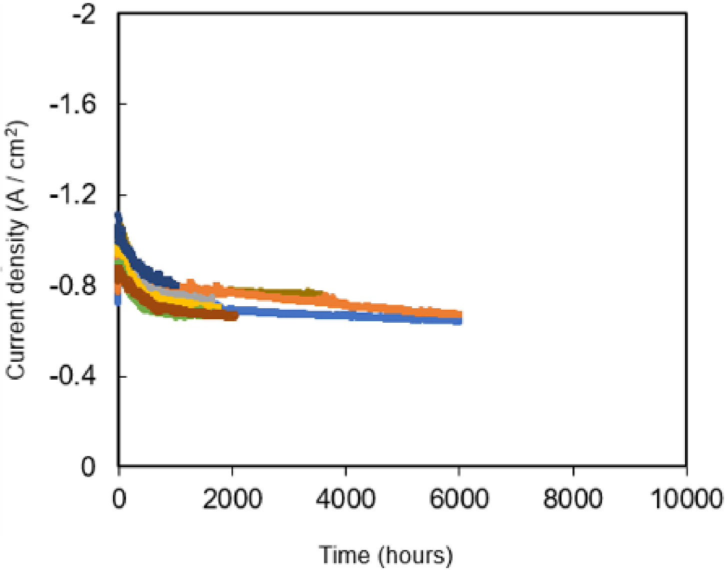
- Relevant steam utilization
- High currents
- Interconnect
- Seals
- Impurities

Multiple cell stack testing

- All stack components
- Assembly issues
- Steam delivery and utilizations
- Heat management
- Durability

Intra and Inter Lab Performance Reproducibility

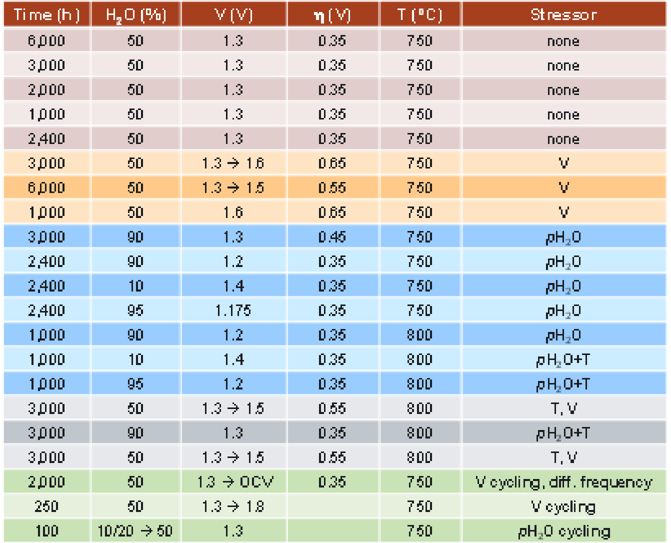




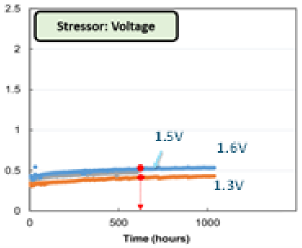
- Established a baseline cell performance for 1,000-6,000 hrs using multiple cells
- Demonstrated performance reproductivity

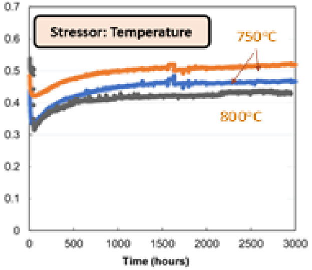
Marina et al., in preparation

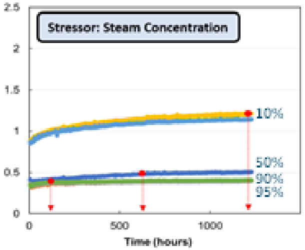
Accelerated Stress Testing to Understand Degradation Mechanisms

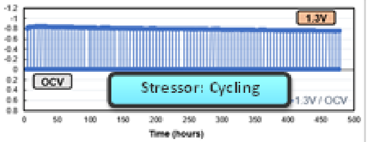


Time (h)	H_2O (%)	V (V)	η (V)	T (°C)	Stressor
6,000	50	1.3	0.35	750	none
3,000	50	1.3	0.35	750	none
2,000	50	1.3	0.35	750	none
1,000	50	1.3	0.35	750	none
2,400	50	1.3	0.35	750	none
3,000	50	1.3 → 1.6	0.65	750	V
6,000	50	1.3 → 1.5	0.55	750	V
1,000	50	1.6	0.65	750	V
3,000	90	1.3	0.45	750	pH_2O
2,400	90	1.2	0.35	750	pH_2O
2,400	10	1.4	0.35	750	pH_2O
2,400	95	1.175	0.35	750	pH_2O
1,000	90	1.2	0.35	800	pH_2O
1,000	10	1.4	0.35	800	pH_2O+T
1,000	95	1.2	0.35	800	pH_2O+T
3,000	50	1.3 → 1.5	0.55	800	T, V
3,000	90	1.3	0.35	800	pH_2O+T
3,000	50	1.3 → 1.5	0.55	800	T, V
2,000	50	1.3 → OCV	0.35	750	V cycling, diff. frequency
250	50	1.3 → 1.8		750	V cycling
100	10/20 → 50	1.3		750	pH_2O cycling









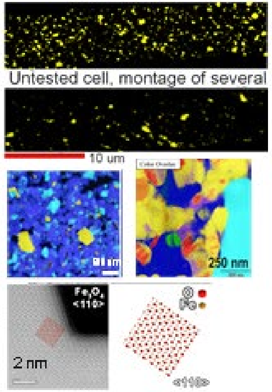
- Established a baseline performance for 1,000-6,000 h
- Completed initial AST using different stressors
- Validated with multiple repeats

Le at el., in preparation

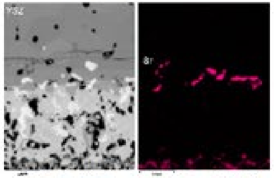
Probing for Degradation Mechanisms: SEM, TEM, APT

Oxygen Electrode Characterization after 3,000 hours

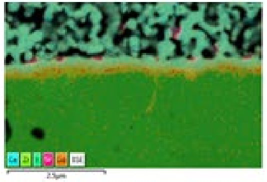
Co inconsistency



Sr migration



Gd diffusion into YSZ

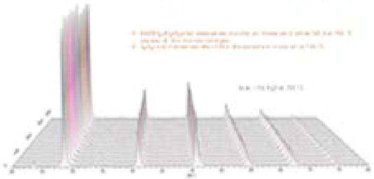


- SEM/EDS
- EBSD
- TEM/STEM
- E-SEM, E-TEM
- HT XRD
- APT

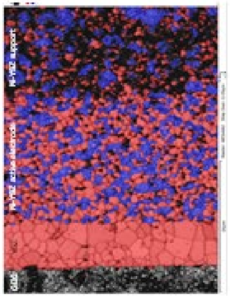
Edwards et al., in preparation

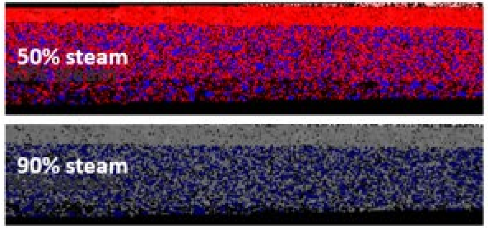
In Operando High Temperature XRD

13 mm ⌀ button cell
Up to 1000°C with different gases and current load

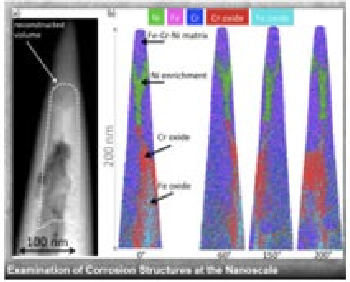


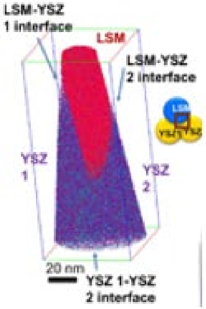
Hydrogen Electrode after 3,000 hours in 90% steam





3D Atom Probe Tomography





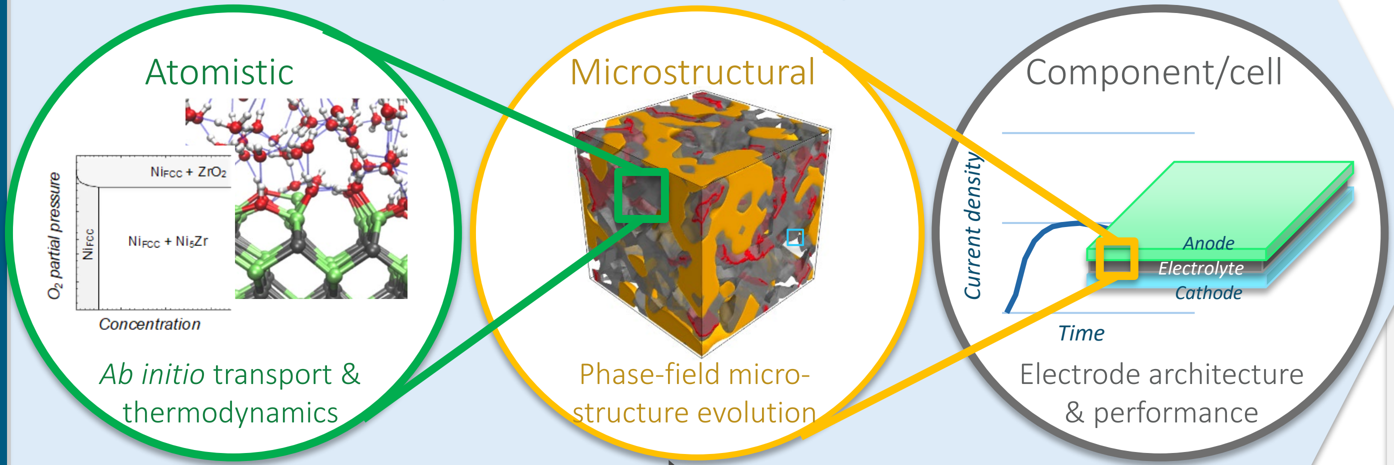
H2NEW Activities: High Temperature Electrolysis (HTE)

Materials Degradation Modeling

H2NEW multiscale modeling strategy for critical degradation modes

"Bottom-up"

Multiscale physics-based modeling of mechanisms



Atomistic

Ab initio transport & thermodynamics

Microstructural

Phase-field micro-structure evolution

Component/cell

Electrode architecture & performance

Models are linked across scales, correlated to testing data, and accelerated with ML/AI

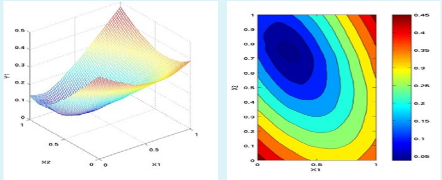
Suggest relevant mechanisms

Suggest testing conditions

"Top-down"

Performance analysis

test matrix → correlations → inferences

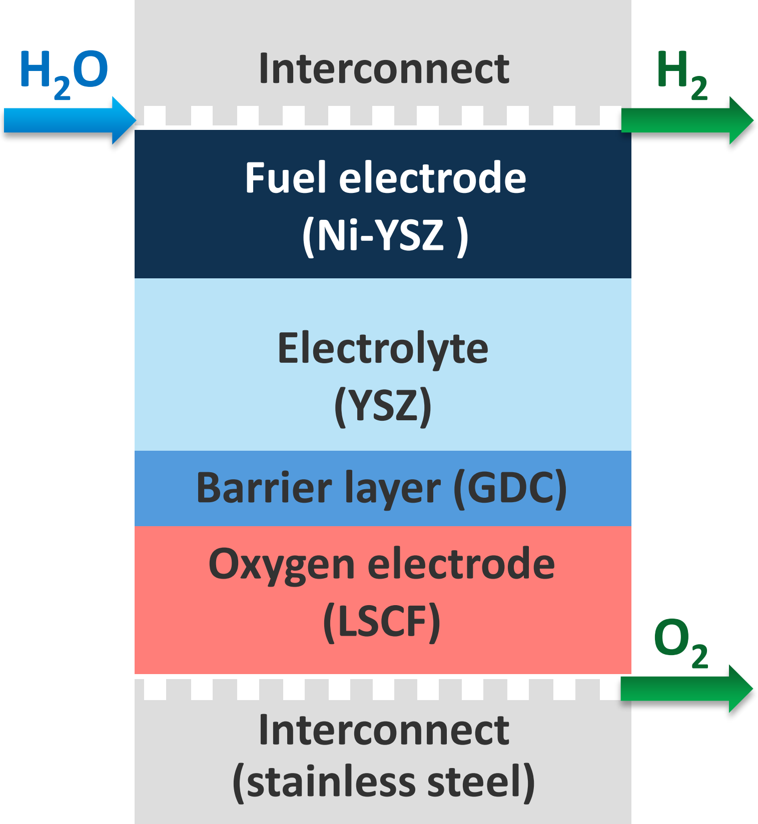


Relevant degradation modes

Materials/ components/ cells

Operating conditions

Models probe multiple degradation mechanisms for solid oxide electrolysis cells



- Interconnect corrosion

- Ni redistribution & coarsening
- Secondary phase formation & particle breakdown

- Cation migration and interdiffusion among electrode, electrolyte, and barrier layer

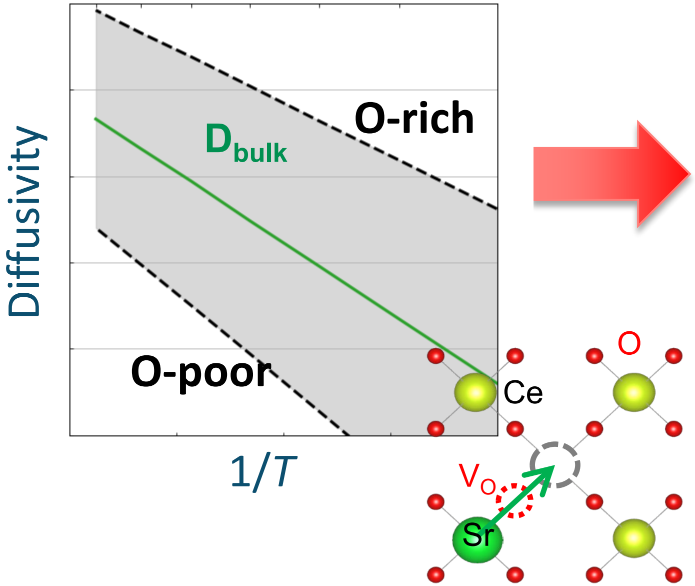
- Electrode decomposition & secondary phase formation

- Interconnect / electrode interactions (Cr poisoning)
- Air electrode mechanical failure

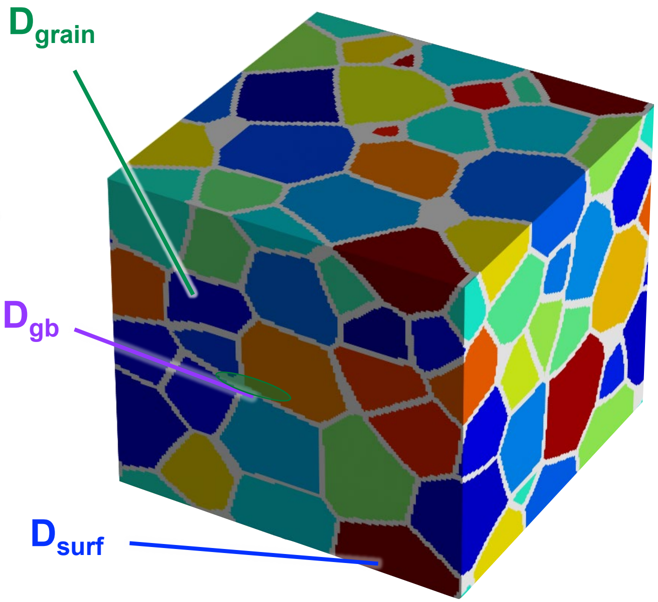
Multiscale integration for physics-based degradation models

Example: Cation diffusion through interlayer

Ab initio diffusivity predictions



"Digital twin" microstructures

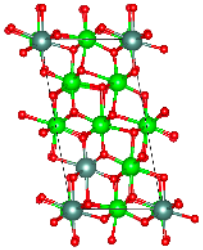


- Models couple ion diffusion to *local* oxygen chemical potential and electrical potential variations
- Strong dependence on microstructure can be incorporated

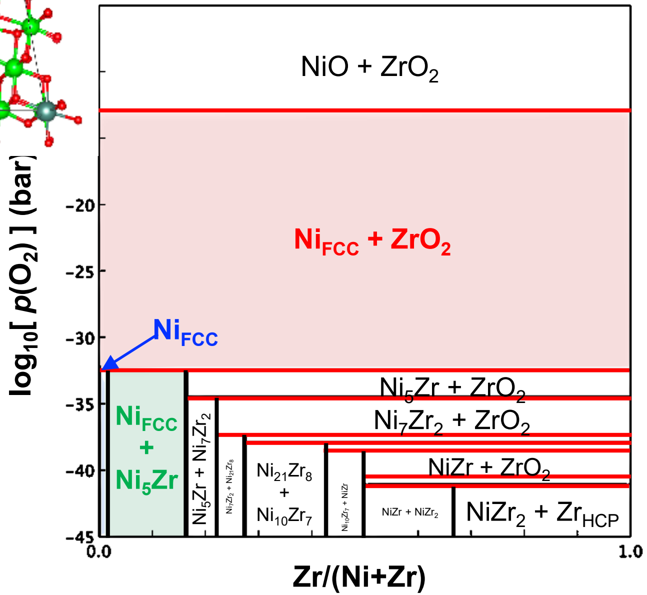
Multiscale integration for physics-based degradation models

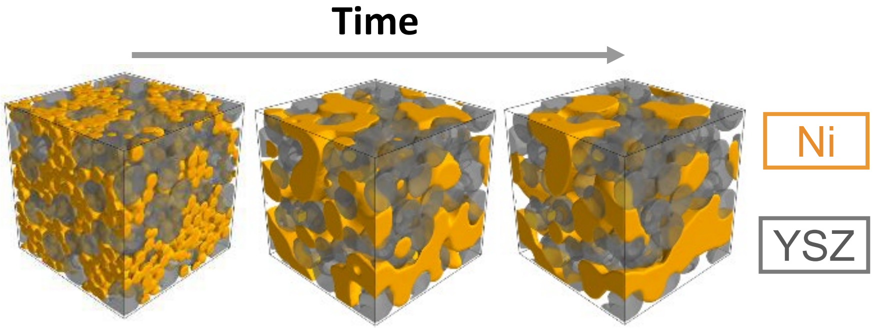
Example: Secondary phase formation at Ni-YSZ interface

YSZ



Ab initio thermodynamic predictions

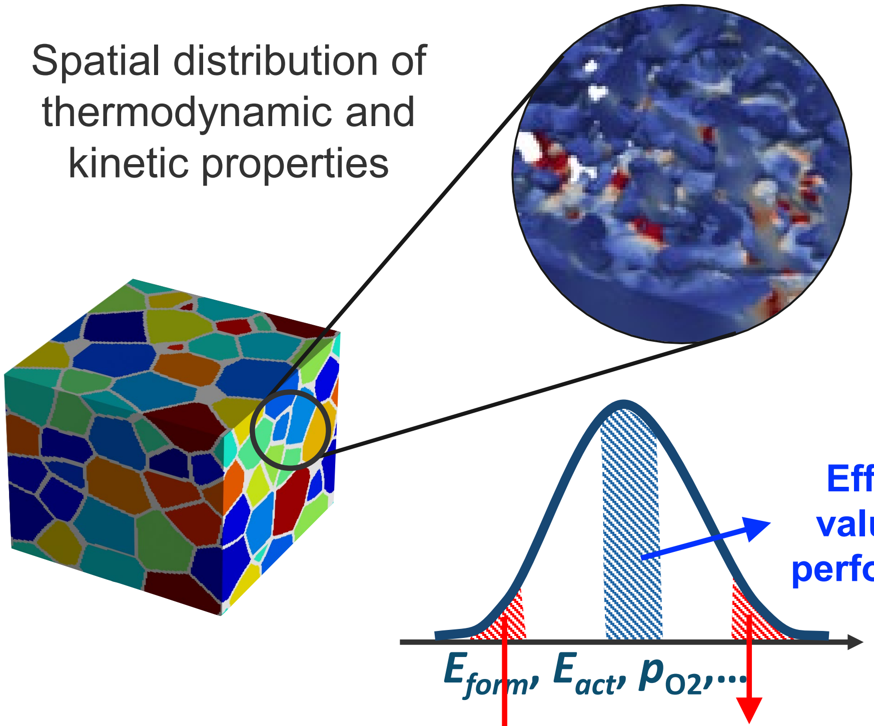




Phase-field model of local phase formation

Statistical approaches for predicting local hotspots and heterogeneous response

Spatial distribution of thermodynamic and kinetic properties

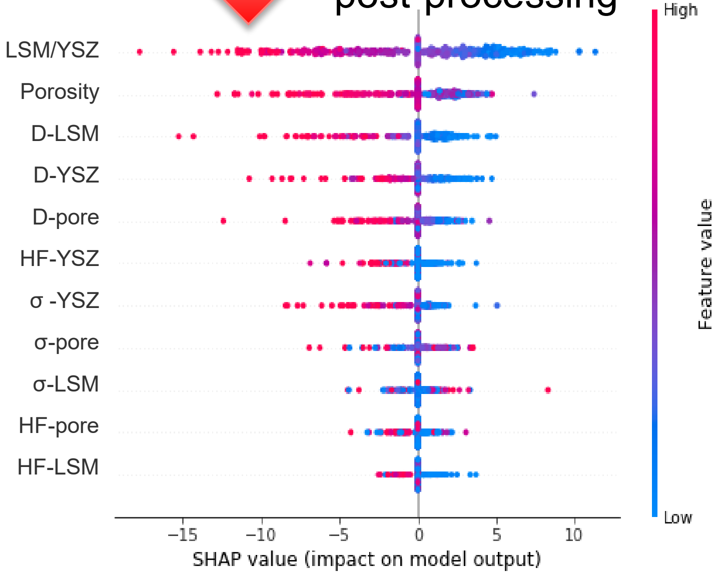


Effective values for performance

Hotspots for degradation

Important features and sensitivities from statistics across thousands of electrode microstructures

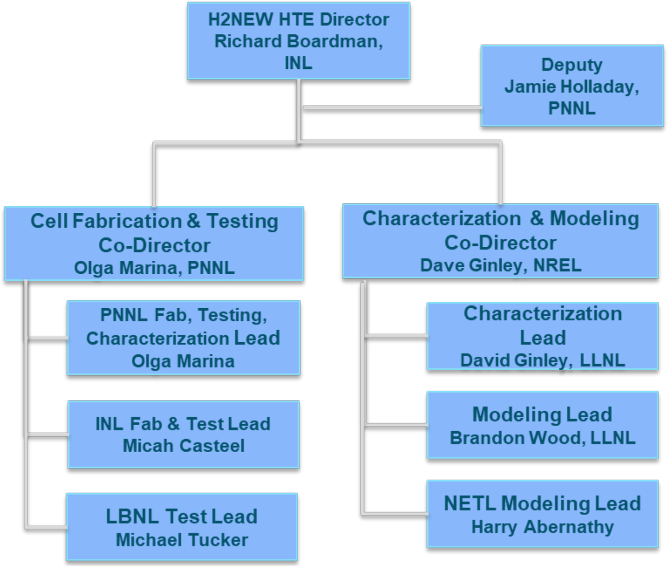
ML-based post-processing



H2NEW Activities: High Temperature Electrolysis (HTE)

Synchrotron SOEC characterization

Integrated characterization & modeling approach



Characterization

- Identification & quantification of degradation as a function of cell aging & operating condition
- Validation of AST protocols
- Data for model development
- Validation of models

⇄

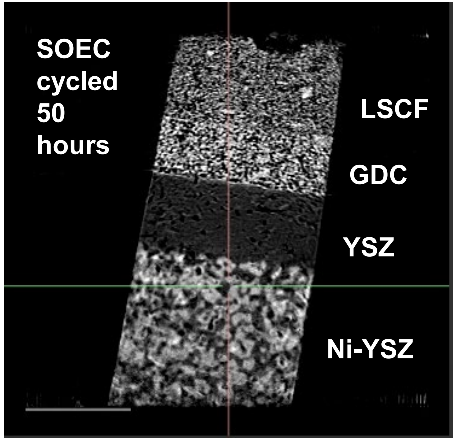
Modeling

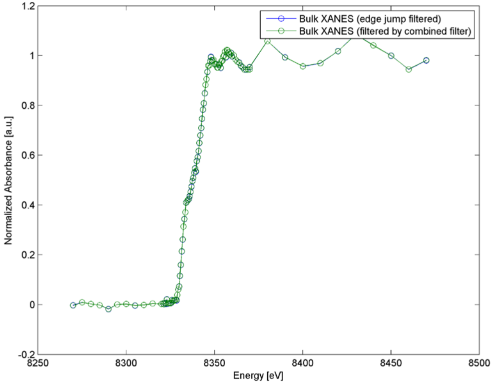
- Mechanistic understanding of degradation & impact on performance
- Results guide characterization objectives & experiment design

Multi-faceted characterization approach from molecular to micron length scales is key

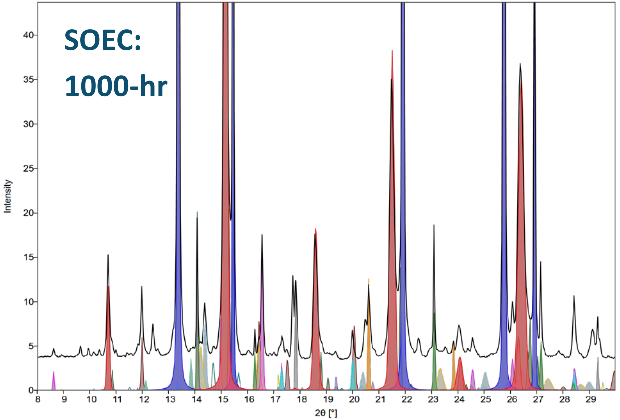
Synchrotron characterization – SOEC degradation

Imaging w/ Spectroscopy





XRD



XRD @ Synchrotron:

- High throughput analysis of **in-tact** button & planar cells
- Depth profiling
- Quantifiable phase identification
- Simultaneous XRF
- In situ

Expected Phases Present

- $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$ (R-3c)
- $Ce_{0.9}Gd_{0.1}O_{1.95}$ (Fm-3m)
- $Zr_{0.8}Y_{0.2}O_{1.9}$ (Fm-3m)
- Ni metal (Fm-3m)
- Ag (Fm-3m) - contact
- Al_2O_3 (R-3cH)

Degradation Products

- $Co_xFe_{3-x}O_4$, Co_3O_4 (Fd-3m) – requires Co reduction
- SrO
- La_2O_3
- $SrZrO_3$ (Pm-3m) – Zr and/or Sr migration
- $La_{1-x}Sr_xCoO_{3-\delta}$
- Tetragonal structures of LSCF

H2NEW Website – Community Resource

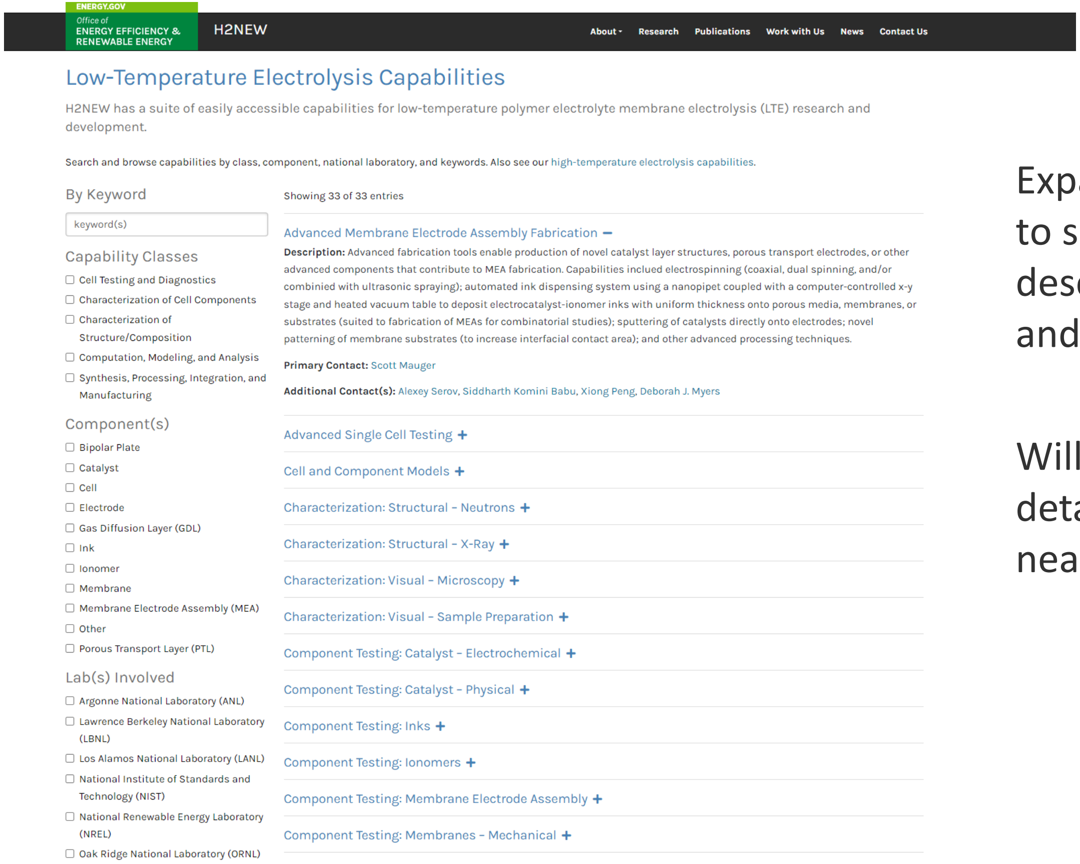
https://h2new.energy.gov/

H2NEW Website - https://h2new.energy.gov

Sorted by LTE and HTE under Research tab in banner

Searchable by Keyword

Sortable by Capability Class, Component and/or Labs involved



Low-Temperature Electrolysis Capabilities

H2NEW has a suite of easily accessible capabilities for low-temperature polymer electrolyte membrane electrolysis (LTE) research and development.

Search and browse capabilities by class, component, national laboratory, and keywords. Also see our high-temperature electrolysis capabilities.

By Keyword

keyword(s)

Capability Classes

- ☐ Cell Testing and Diagnostics
- ☐ Characterization of Cell Components
- ☐ Characterization of Structure/Composition
- ☐ Computation, Modeling, and Analysis
- ☐ Synthesis, Processing, Integration, and Manufacturing

Component(s)

- ☐ Bipolar Plate
- ☐ Catalyst
- ☐ Cell
- ☐ Electrode
- ☐ Gas Diffusion Layer (GDL)
- ☐ Ink
- ☐ Ionomer
- ☐ Membrane
- ☐ Membrane Electrode Assembly (MEA)
- ☐ Other
- ☐ Porous Transport Layer (PTL)

Lab(s) Involved

- ☐ Argonne National Laboratory (ANL)
- ☐ Lawrence Berkeley National Laboratory (LBNL)
- ☐ Los Alamos National Laboratory (LANL)
- ☐ National Institute of Standards and Technology (NIST)
- ☐ National Renewable Energy Laboratory (NREL)
- ☐ Oak Ridge National Laboratory (ORNL)

Showing 33 of 33 entries

Advanced Membrane Electrode Assembly Fabrication −

Description: Advanced fabrication tools enable production of novel catalyst layer structures, porous transport electrodes, or other advanced components that contribute to MEA fabrication. Capabilities inclued electrospinning (coaxial, dual spinning, and/or combinied with ultrasonic spraying); automated ink dispensing system using a nanopipet coupled with a computer-controlled x-y stage and heated vacuum table to deposit electrocatalyst-ionomer inks with uniform thickness onto porous media, membranes, or substrates (suited to fabrication of MEAs for combinatorial studies); sputtering of catalysts directly onto electrodes; novel patterning of membrane substrates (to increase interfacial contact area); and other advanced processing techniques.

Primary Contact: Scott Mauger

Additional Contact(s): Alexey Serov, Siddharth Komini Babu, Xiong Peng, Deborah J. Myers

Advanced Single Cell Testing +

Cell and Component Models +

Characterization: Structural – Neutrons +

Characterization: Structural – X-Ray +

Characterization: Visual – Microscopy +

Characterization: Visual – Sample Preparation +

Component Testing: Catalyst – Electrochemical +

Component Testing: Catalyst – Physical +

Component Testing: Inks +

Component Testing: Ionomers +

Component Testing: Membrane Electrode Assembly +

Component Testing: Membranes – Mechanical +

Expandable/collapsible to show high level descriptions, primary and additional contacts.

Will add link to more detailed descriptions in near future.