FC171

Advanced PGM-free Cathode Engineering for High Power Density and Durability

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Pittsburgh, PA

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DE-EE0008076

Overview

Timeline and Budget

- Project Start Date: 09/01/2017
- Project End Date: 08/31/2020
- Total Project Budget: $2,292,324
  - Total Recipient Share: $292,324
  - Total Federal Share: $2,000,000
  - Total DOE Funds Spent*: $120,700

    * As of 03/31/2018

Barriers

B. Cost

➢Reduce PEM fuel cell costs by replacing precious metal catalysts with PGM-free catalysts

C. Performance

➢Increase catalyst activity, utilization, and effectiveness to enable high fuel cell power density operation

A. Durability

➢Increase stability of PGM-free catalysts at relevant fuel cell voltage

Project Lead

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- PI: Shawn Litster
- Co-PI: Venkat Viswanathan
- Co-PI: Reeja Jayan

Partners

University at Buffalo, SUNY

- PI: Gang Wu

Giner, Inc.

- PI: Hui Xu

3M Company

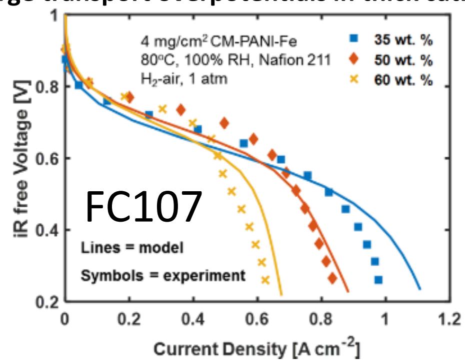
- PI: Andrew Haug

Electrocatalysis Consortium Members

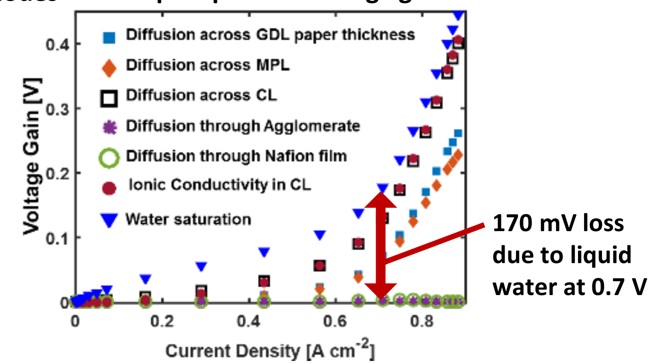
Challenges: PGM-free Cathode Performance and Durability

- Fe-doped MOF-based catalysts have shown promising activity and stability at 0.7 V during fuel cell operation
- Further increases in activity and stability are required to meet performance targets
- Electrode-scale transport losses significantly hinder PGM-free catalyst effectiveness due to ~10X greater cathode thickness resulting from lower volumetric activity
- Significant liquid water flooding and ohmic losses need to be addressed to realize PGM-free ORR activity measured by RDE in a fuel cell MEA
- Prior transport and MEA model analyses in FC107 (PI: Zelenay, LANL) showed gains in power density could be achieved by porous electrode engineering that are comparable to order of magnitude increases in active site density

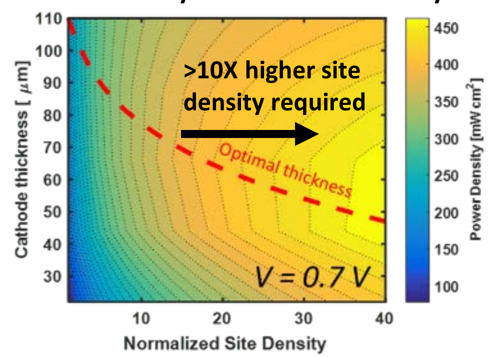
Large transport overpotentials in thick cathodes



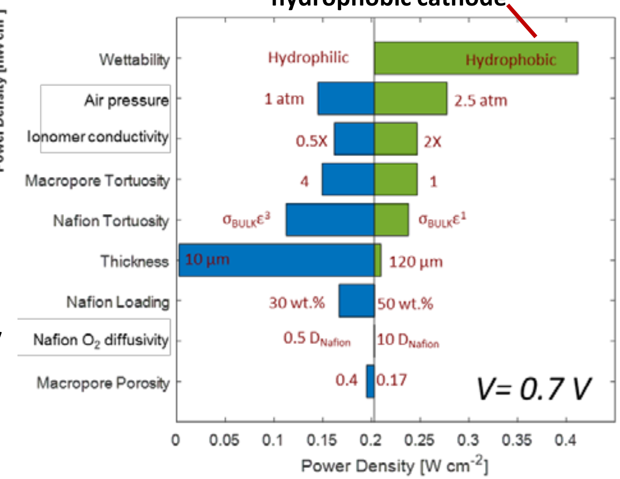
Transport process voltage gain



Power density vs. active site density

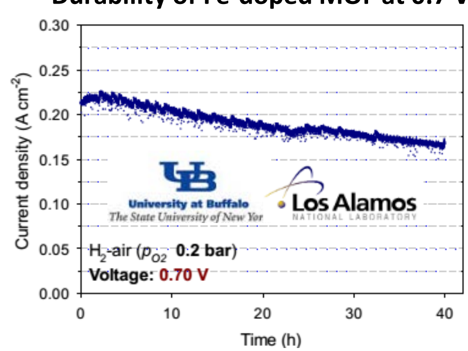


>100% increase in power density with hydrophobic cathode



Komini Babu et al., *J. Electrochem. Soc.*, 2017.

Durability of Fe-doped MOF at 0.7 V



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Technical Targets and Status

Property	DOE 2020 target	Present project status	Project end goal
PGM-free catalyst activity (voltage at 0.044 A/cm²)	0.9 $V_{IR\text{-}free}$	0.87 $V_{IR\text{-}free}$ [a]	>0.9 $V_{IR\text{-}free}$
Loss in initial catalyst mass activity	PGM: <40 %	-	<50%
Loss in performance at 0.8 A/cm²	PGM: <30 mV	-	<50 mV
MEA performance @ 0.8 V	PGM: 300 mA/cm²	63 mA/cm²	>150 mA/cm²
MEA performance @ rated voltage (150 kPa_{abs})	PGM: 1000 mW/cm²	154 mW/cm² at 0.7 V	Stretch goal: >450 mW/cm² at 0.7 V

[a] Pre-project testing of UB Fe-MOF catalyst hand painted CCM at LANL

Objectives

- Enable high, durable power density with new cathode designs specifically for PGM-free catalysts
- Increase PGM-free catalyst activity and stability through synthesis using a simplified, low cost method
- Improve PGM-free mass activity through optimization of the ionomer integration
- Mitigate PGM-free cathode flooding for fast oxygen transport across thick electrodes

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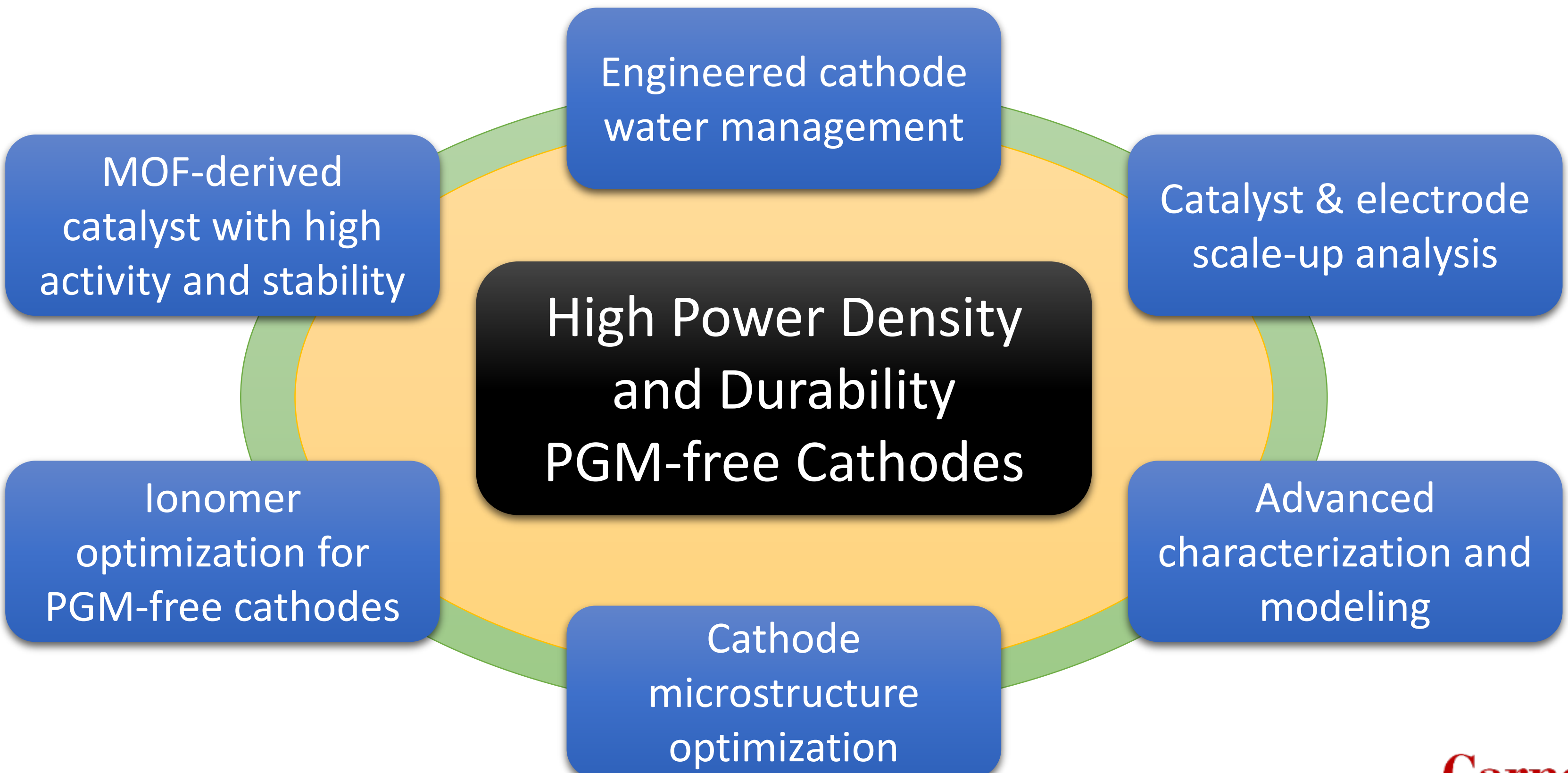
Overview

1. Stable, high activity MOF-derived M-N-C catalysts (M = Fe, Co)
2. PGM-free cathode engineering for enhanced transport and catalyst utilization
3. Ionomer optimization for PGM-free cathodes



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Approach

Year 1 & 2 Milestones and Go/No-Go Points

Milestone or GNG No.	Description	% complete	Notes
Q1 M1.1	State of the art (SOA) PGM-free catalyst synthesized and 2 g delivered to CMU for initial electrode development.	100%	Catalysts have been synthesized and supplied as needed to CMU.
Q2 M1.2	The optimized catalyst demonstrates a half-wave potential **$E_{½}$ ≥ 0.85 V vs. RHE** in acidic electrolyte (RDE test) and generates a current density of **0.5 mA/cm² at 0.90 $V_{IR\text{-}free}$** (RDE test).	100%	Achieved **E½ = 0.87 V *vs.* RHE** in acidic electrolyte (RDE test) and generates a current density of **1.5 mA/cm² at 0.90 $V_{IR\text{-}free}$** (RDE test) at a high loading.
Q3 M2.1	BOL MEA power density of **240 mW/cm² at 0.7 V** with 150 kPa abs backpressure, 100% RH in H_2/air and at a cell temperature of 80°C.	65%	In progress. Currently at 154 mW/cm² at 0.7 V .
Q4 G1	Go/No-Go Decision Point: Demonstrate **$E_{½}$ ≥ 0.86 V vs. RHE** (RDE test) and **0.75 mA/cm² at 0.90 $V_{IR\text{-}free}$** (RDE test). Demonstrate **$\Delta E_{½}$ < 20 mV after 30,000 potential cycles** (0.6 to 1.0 V, 50 mV/s) in O_2 saturated H_2SO_4. For MEA, demonstrate **≥20 mA/cm² at 0.90 V (iR-corrected) in an H_2-O_2** fuel cell with an O_2 partial pressure of 1.0 bar at 80 °C.	60%	The RDE E½ and ORR current density G1 targets have been achieved with a catalyst having a 26 mV drop after 30,000 cycles, which is close to target of <20 mV. In MEAs, 20 mA/cm² has been achieved at 0.88 V (O_2/H_2).
Q5 M3.1	**Activity and stability as a function of ionomer type, EW, and loading**. Down select ionomers that provide >5 mV increase in half-wave potential and higher bulk conductivity.	30%	Ionomer testing underway.
Q6 M2.2	CMU model results for synthesis targets and electrode optimization based on imaging and characterization of SOA catalysts. Provide **target active site density and cathode thickness** to meet project end goal.	30%	CMU modeling being updated for UB catalyst morphology and kinetics.
Q7 M2.3	Demonstrate **30% increase in MEA limiting current density** through improved water management by hydrophobic support layers or iCVD treatment while **current density is >100 mA/cm² at 0.8 V** (150 kPa abs backpressure, 100% RH H2/air at a cell temperature of 80˚C)	25%	Hydrophobic support and iCVD coating methods in development.
Q8 G2	Demonstrate **≥25 mA/cm² at 0.90 V** (iR-corrected) in an H_2-O_2 fuel cell with an O_2 partial pressure of 1.0 bar (cell temperature 80 °C). Voltage loss at 0.044 A/cm² less than 100 mV after 30,000 voltage cycles (0.6 to 1.0 V) under H_2-N2 condition.	20%	In progress. Currently 25 mA/cm² at 0.873 $V_{IR\text{-}Free}$.

*iR-free voltage is cell voltage corrected for the high frequency resistance (HFR)

Collaborative Project Team

Carnegie Mellon University (University prime)

Prof. Shawn Litster (PI), Dr. Aman Uddin, Lisa Langhorst, Shohei Ogawa, Leiming Hu, Yuqi Guo, Prof. Venkat Viswanathan (co-PI), Gurjyot Sethi, Prof. Reeja Jayan (co-PI), Laisuo Su

Electrode design, hydrophobicity treatments, electrode fabrication, fuel cell testing, X-ray imaging, multi-scale modeling, project management.

University at Buffalo-SUNY (University sub)

Prof. Gang Wu (UB PI), Hanguang Zhang, Mengjie Chen, Hao Zhang

Catalyst development, synthesis, and experimental characterization.

Giner, Inc. (Industry sub)

Dr. Hui Xu (Giner PI), Shuai Zhao

Catalyst and MEA fabrication scale-up analysis and demonstration, fuel cell testing, support of hydrophobic cathode development.

3M Company (Industry sub)

Dr. Andrew Haug (3M PI)

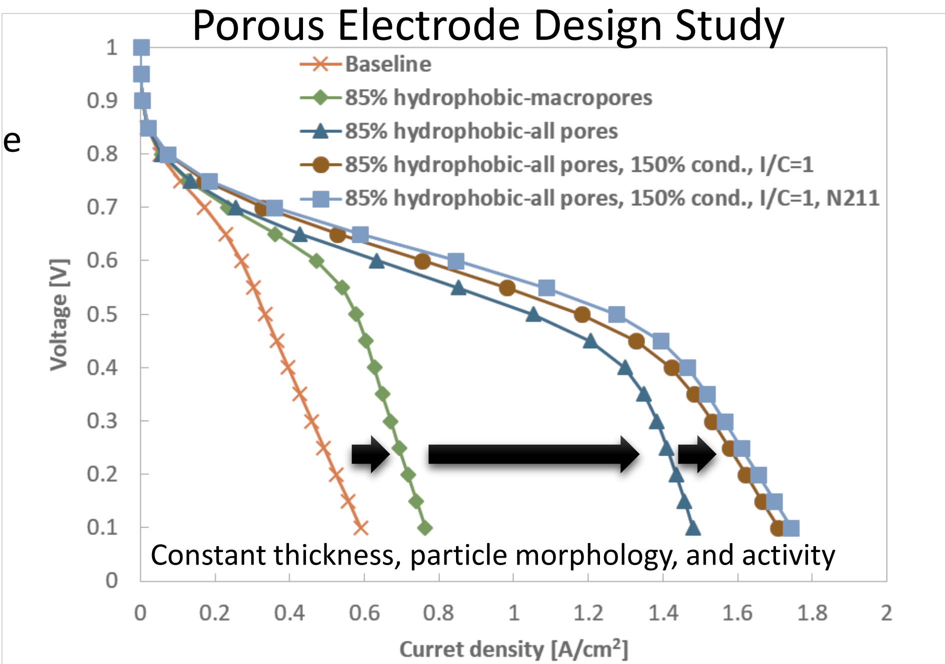
Ionomer supply and optimization support.

Electrocatalysis (ElectroCat) EMN Consortium Members (National Laboratories)

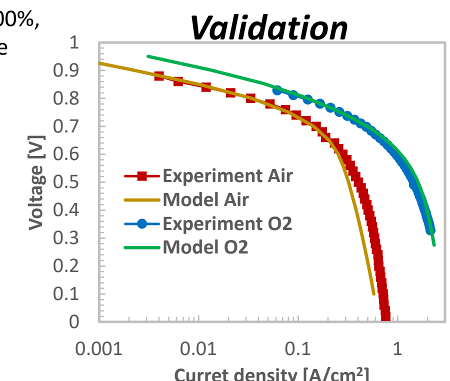
X-ray absorption spectroscopy (ANL), electron microscopy (ORNL), molecular probes studies (LANL & ANL), electrode development (NREL), fuel cell durability testing (LANL).

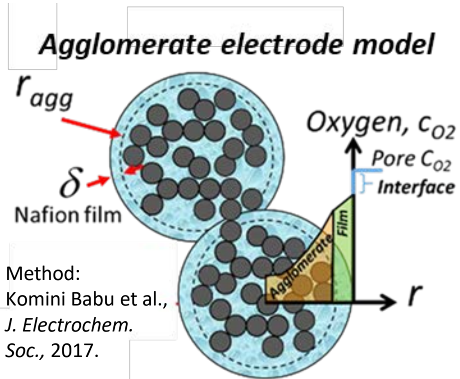
Model-based Road Map to Higher Power Density

- Development of a well-validated multi-phase MEA model with cathode microstructure inputs
- Inputs relating catalyst synthesis to performance include active site density and activity, bimodal particle-size distribution, and pore-size distribution for both secondary and primary pores
- Actionable predictions to inform synthesis
- Significant performance improvement possible by electrode engineering, including increased hydrophobicity and ionomer conductivity
- Optimal cathode thickness versus active site density
- Predicted gains in power density at 0.7 V by electrode engineering are comparable to 4X increase in active site density

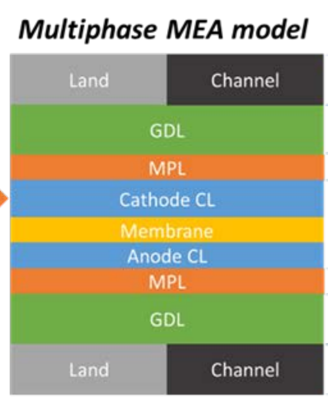


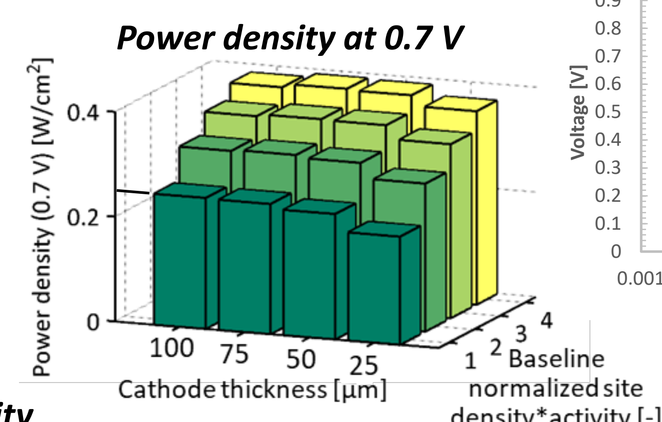
Cell temperature: 80°C; RH: 100%, 1 bar H_2/air-O_2 partial pressure





Method: Komini Babu et al., *J. Electrochem. Soc.*, 2017.





Input of active site density in carbon & single site activity

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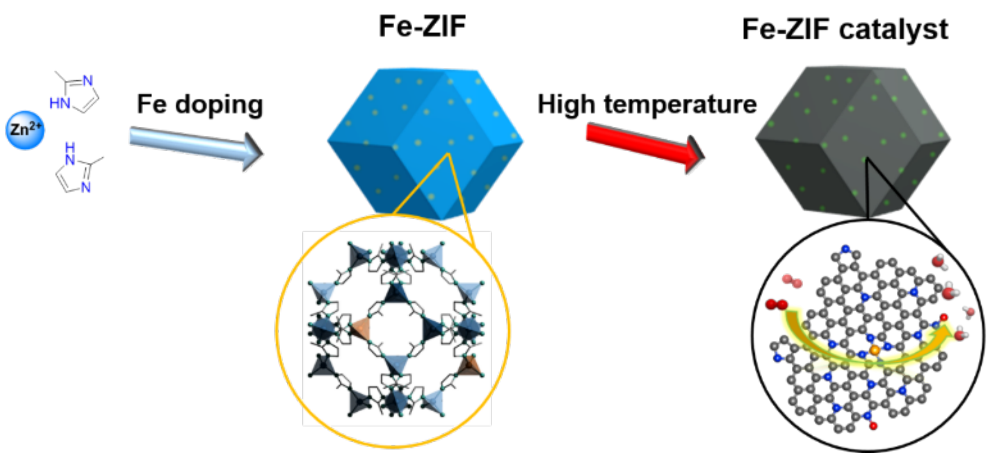
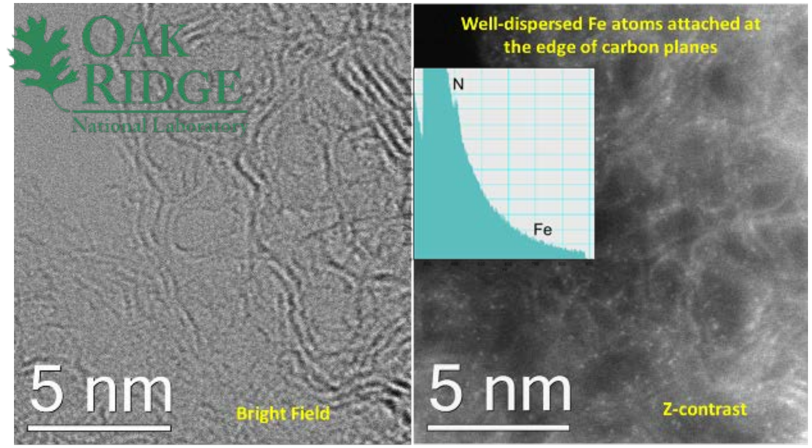
Synthesis of Fe-MOF derived PGM-free catalysts

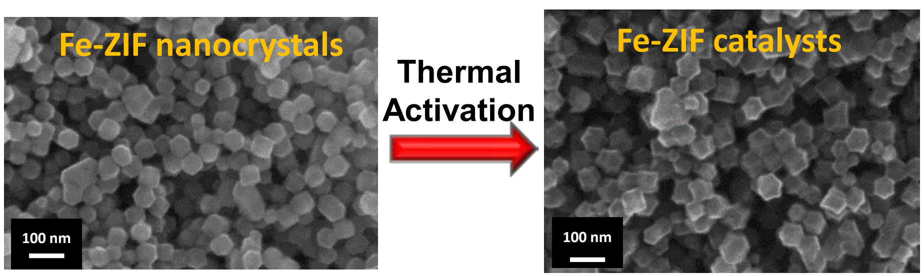
Chemically doped Fe into ZIFs with tunable Fe content



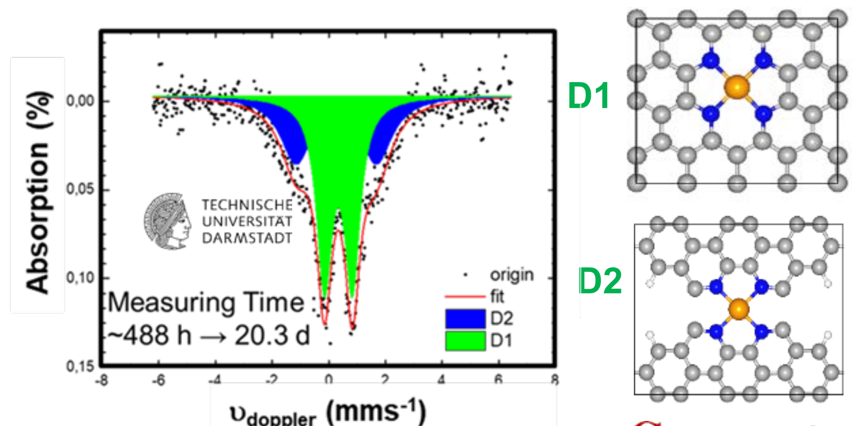
Atomically dispersed Fe sites coordinated with N



Uniform particle dispersion morphology



Exclusive FeN_4 sites in two forms



- Facile and scalable synthesis omitting multistep post-treatments
- Tunable morphology and composition of catalysts from well-defined MOF nanocrystal precursors

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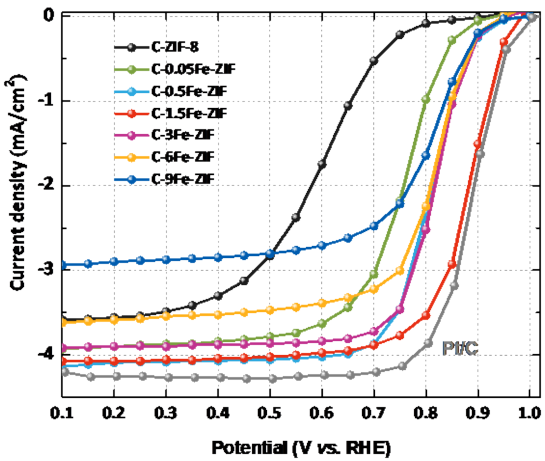
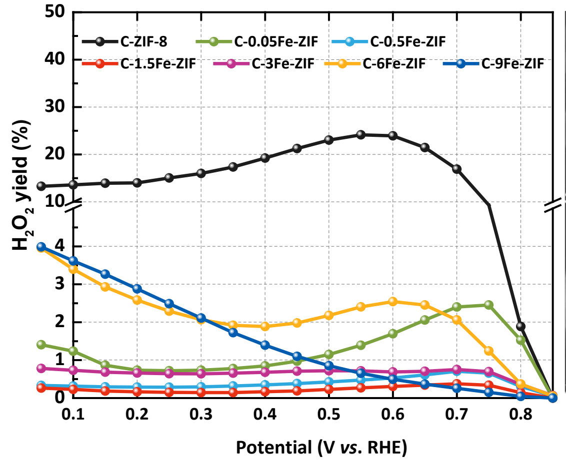
Effect of Fe Doping Content

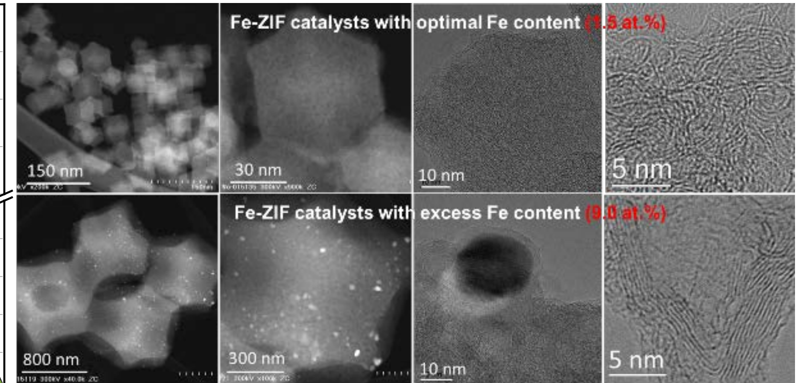
Activity



Selectivity



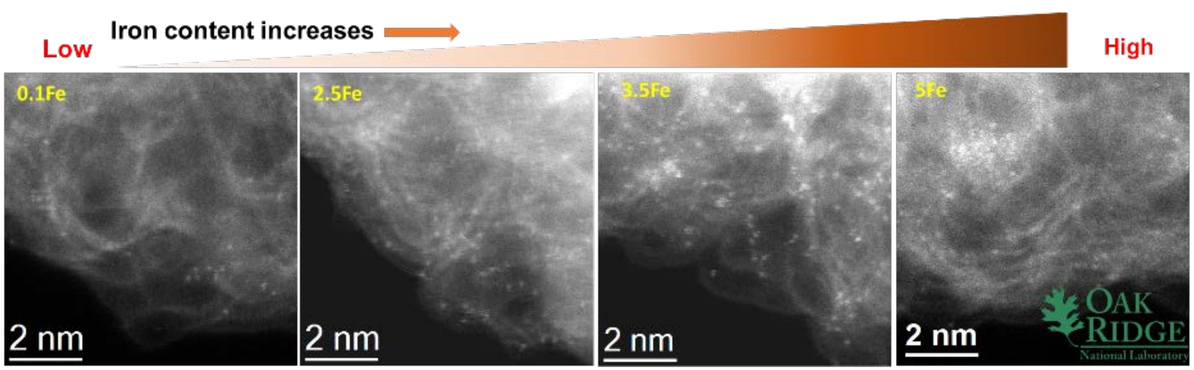
Carbon catalyst microstructures



RRDE: 0.8 mg/cm², 25°C, 900 rpm, 0.5 M H_2SO_4; staircase from 1.05 to 0 V with a step of 0.05 V for 30 s.

Activity/Selectivity: $E_{1/2}$ > 0.85 V; H_2O_2 yield <1%; J > 0.5 mA/cm² at 0.90 V

Evolution of Fe Clustering



- Highly dispersed Fe atoms observed at low iron content, boosting the ORR activity; clusters appear at high iron contents
- Increased Fe content leads to larger carbon particle sizes and causes Fe aggregates that is negative for the ORR in acids
- Highly graphitized carbon microstructures resulted from these iron aggregates is not favorable for activity enhancement, but beneficial for stability improvement

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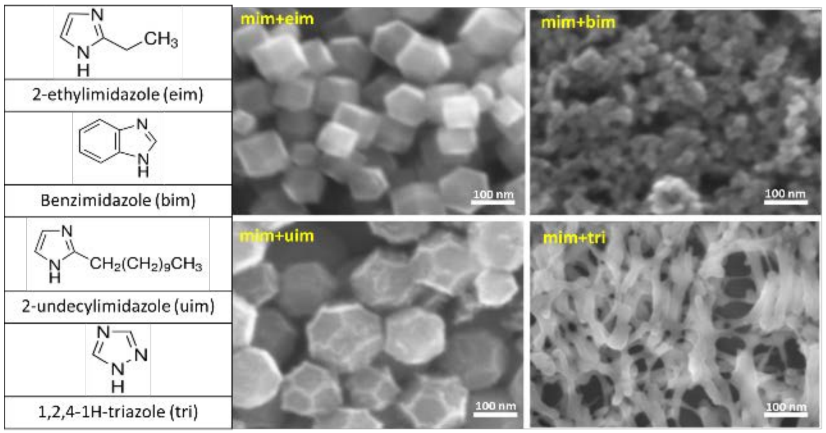
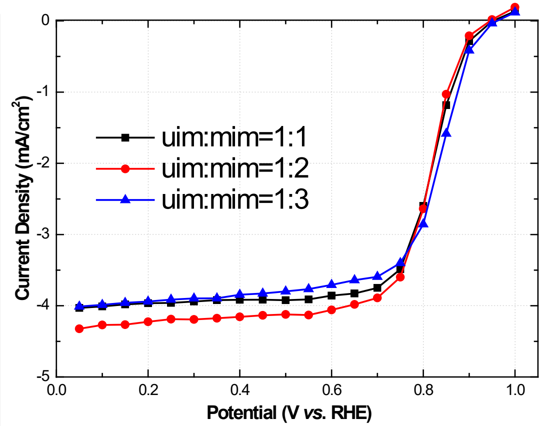
Engineering Morphology by Using Binary Ligands

Binary ligands: 2-methylimidazole (mim) plus the secondary ligand

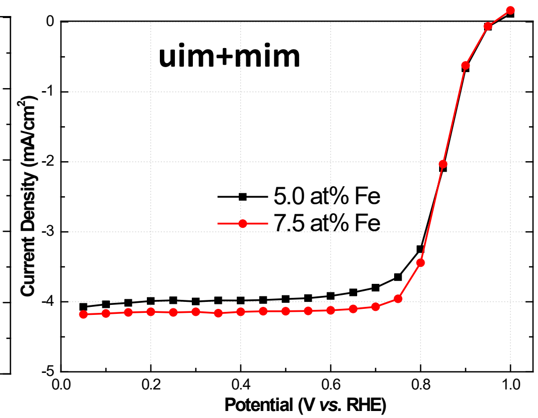
Tunable catalyst morphology



Ratios of binary ligands

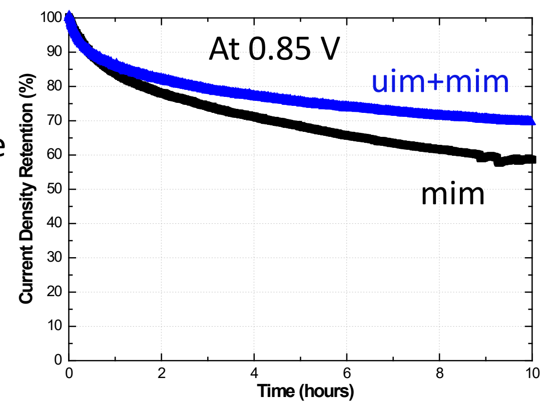


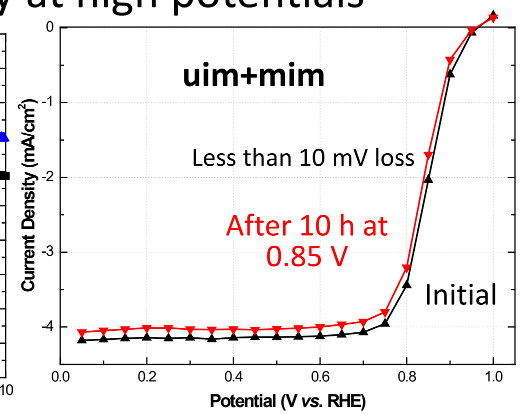
Allow high Fe content



- Engineering catalyst morphology by using binary ligands to synthesize various Fe-MOF nanocrystal precursors
- The uim+mim binary ligand derived catalysts accommodate higher Fe content (7.5 at%) relative to single ligand (mim, 2.5 at%), which potentially increases the density of active sites and stablizes carbon structures in PGM-free catalysts
- The binary ligand-derived catalyst has exhibited promising stability enhancement especially at challenging high potential (i.e. 0.85 V), likely due to improved carbon corrosion resistance

Enhanced stability at high potentials





RDE: 0.8 mg/cm^2, 25°C, 900 rpm, 0.5 M H_2SO_4; holding potential from 1.05 to 0 V with a step of 0.05 V for 30 s.

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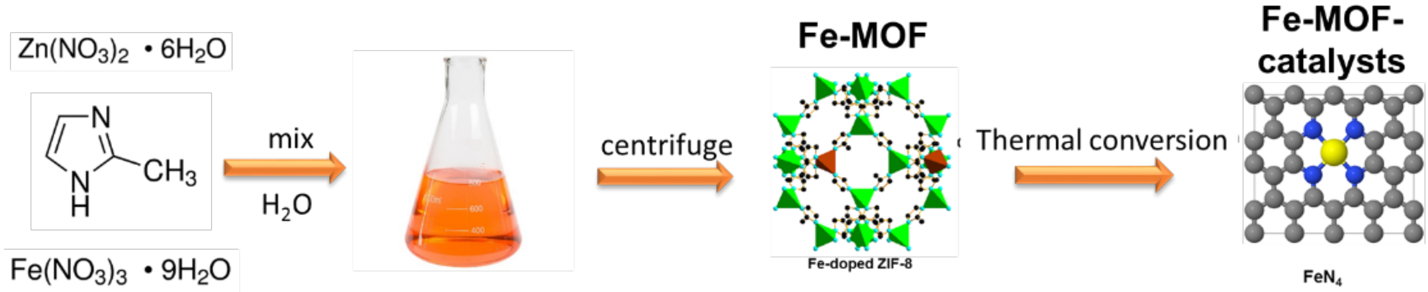
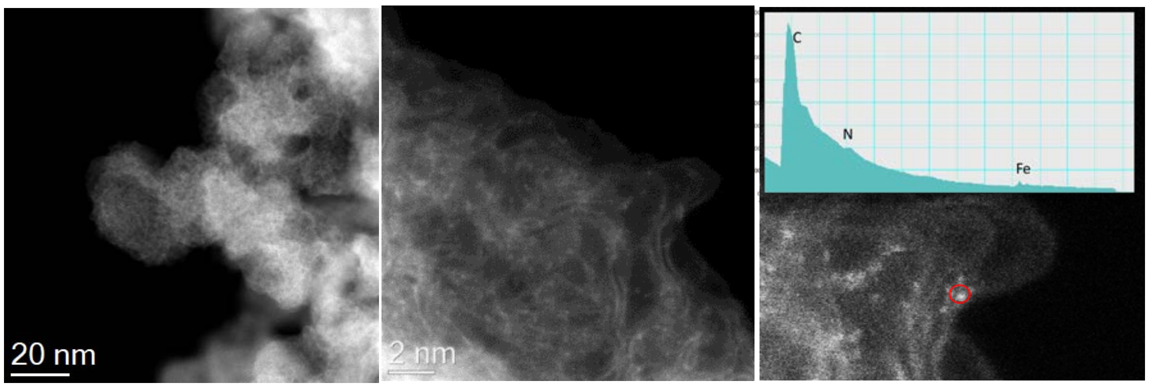
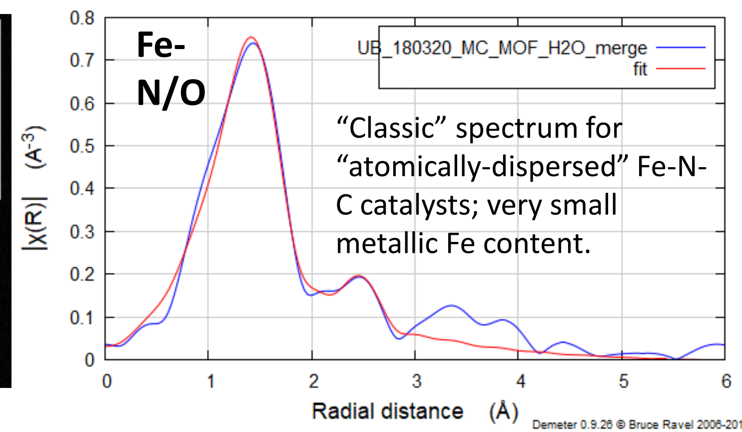
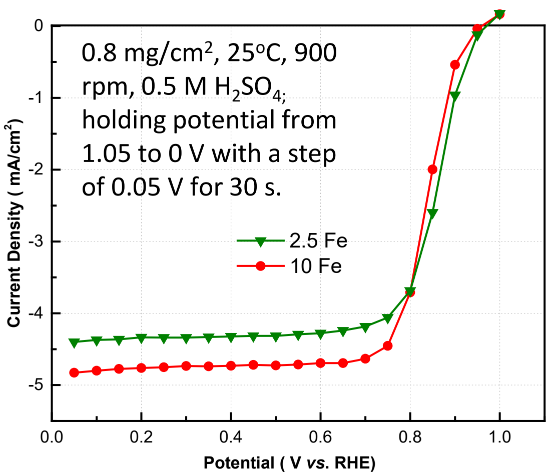
Alternative Green Synthesis Using Water



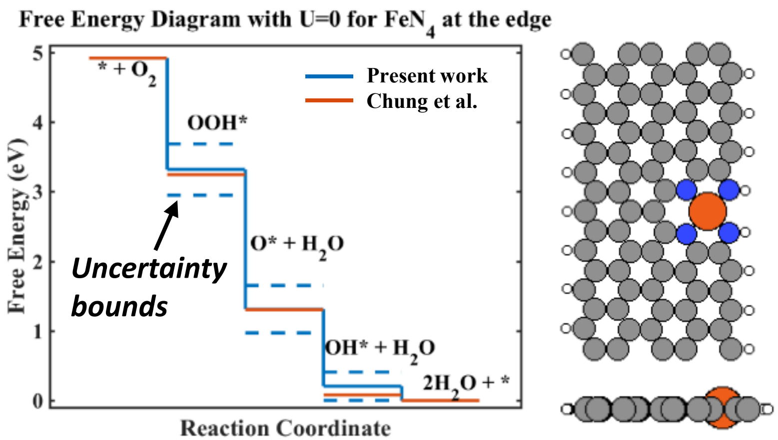




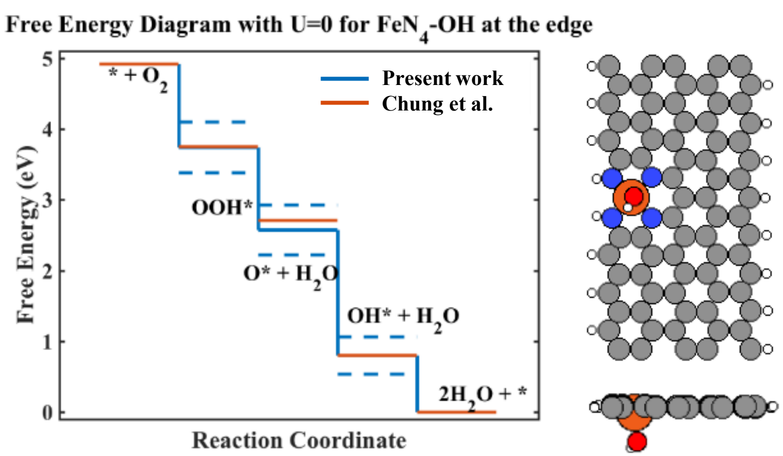


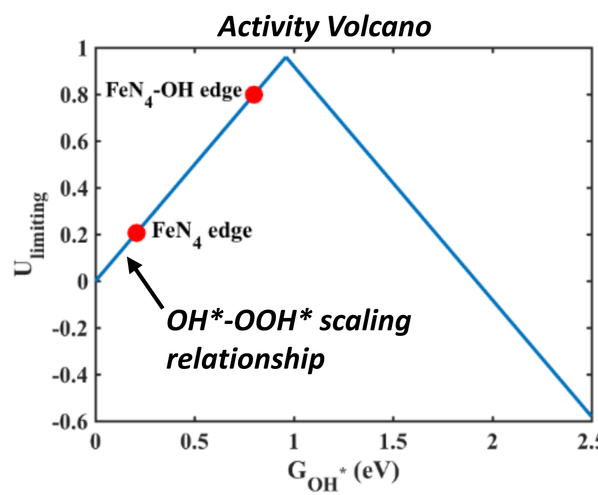
- Environmentally friendly synthesis using aqueous solution rather than organic solvents to prepare atomically dispersed Fe-MOF catalysts
- Unlike traditional MeOH approach, Fe content can be increased up to 10 at% without the formation of clusters, showing comparable activity to low-Fe content (2.5 at%) catalyst
- Water-based synthesis provide an effective strategy to disperse more atomic Fe sites and enhance catalyst stability

Active Site ORR Free Energy diagrams with Uncertainty Quantification



- Free energy diagrams are computed using first principles calculations using the density functional theory (DFT) framework
- BEEF-vdW exchange correlation functional allows the estimation of experimental uncertainty by training the parameters of the functional form on experimental data
- Results from Chung et al. are benchmarked in present work using this functional to validate framework for future studies
- Simulation shows that the edge hosted FeN_4 site with OH ligand has the highest thermodynamic limiting potential
- Activity volcano displays the limiting potential as a function of OH* adsorption energy for the cases considered, presenting expected OH*-OOH* scaling





Chung et al., 2017 *Science*, *357*(6350), pp.479-484.

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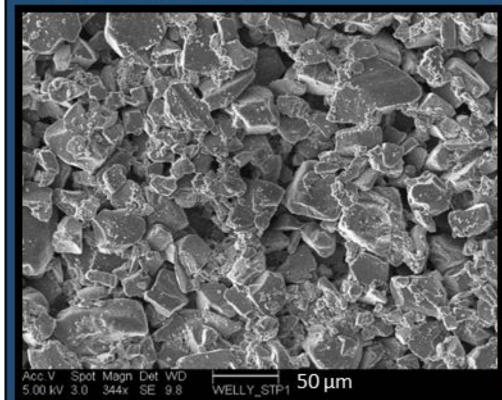
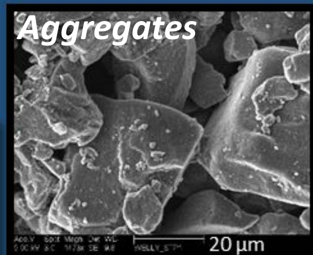
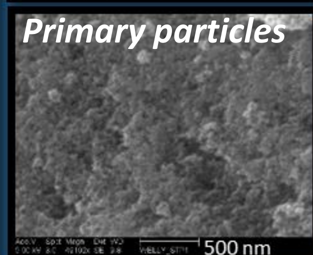
MEA: Particle and Electrode Morphology

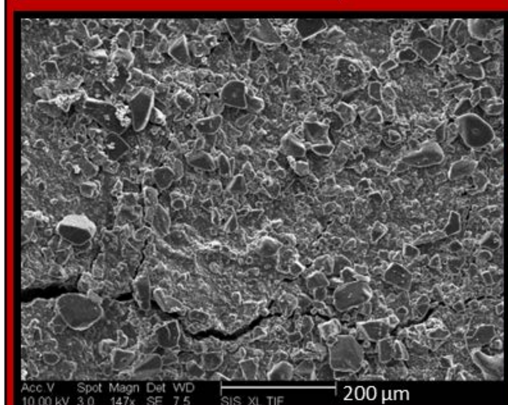
Large fused aggregates of narrow size distribution with large macropores

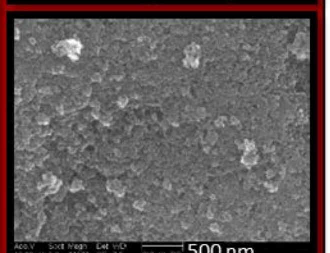






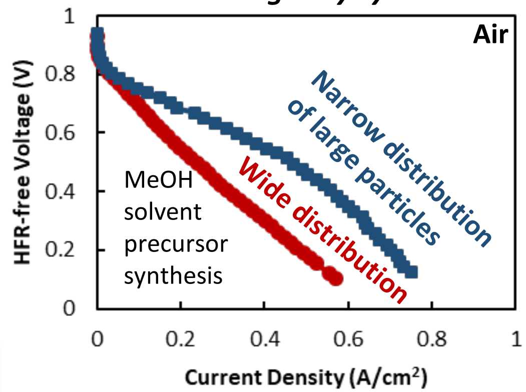
Agglomerated small particles and large fused aggregates of wide size distribution



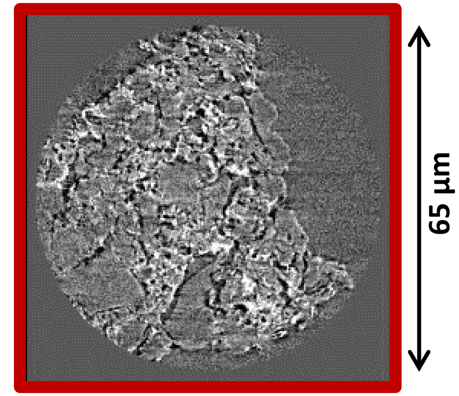


- Variation in aggregate size distribution impacts flooding
- Large aggregates and pores reduce flooding
- Wide aggregate size distributions with smaller aggregates filling large pores form dense electrodes that severely flood
- Primary particle size has a significant impart on performance

Distribution changes by synthesis

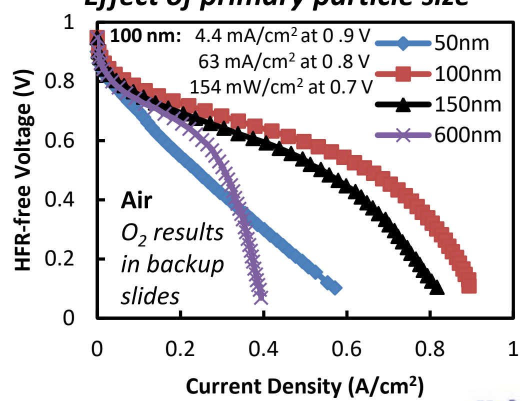


Zernike phase contrast nano-CT of particle-pore morphology

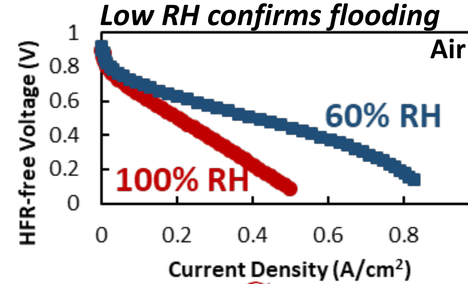


Large field of view: 65 nm voxels

Effect of primary particle size



Low RH confirms flooding



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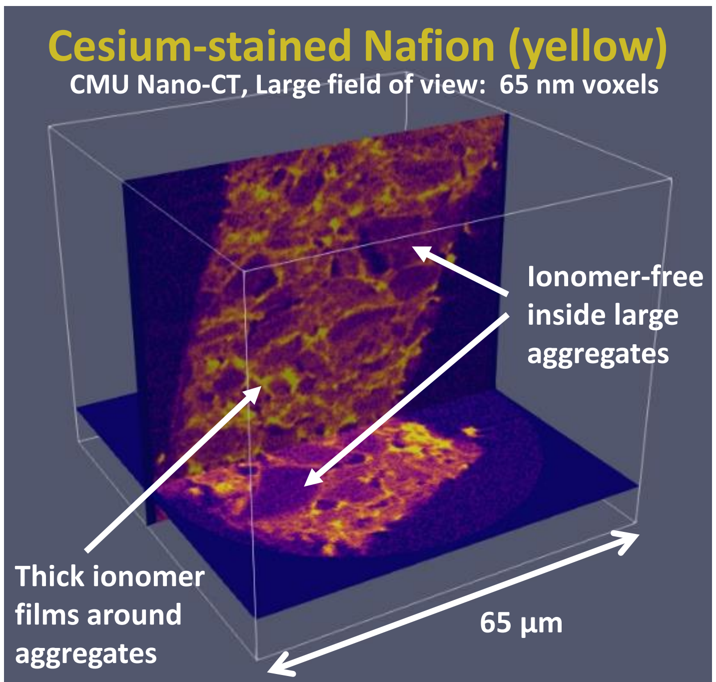
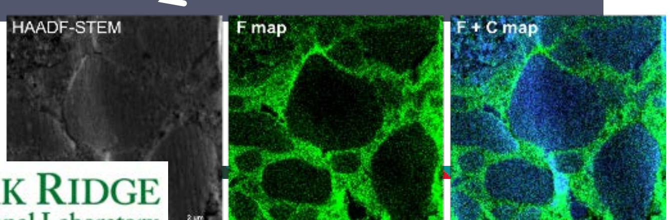
Catalyst loading: 4 mg/cm^2, Cell temperature: 80°C; Flow rate H_2/air: 200/200 sccm
RH: 100%, 1 bar H_2/air partial pressure. Nafion 212

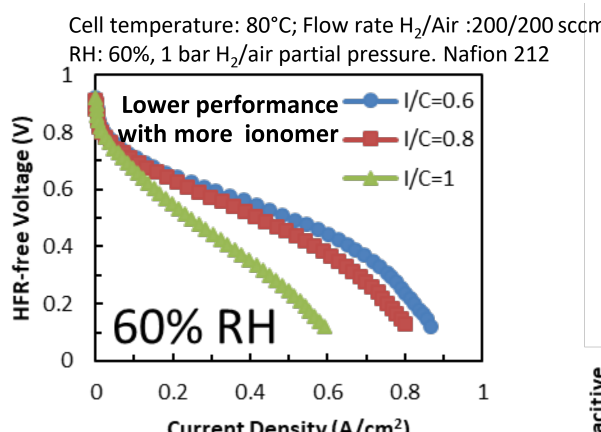
Cathode Ionomer Integration

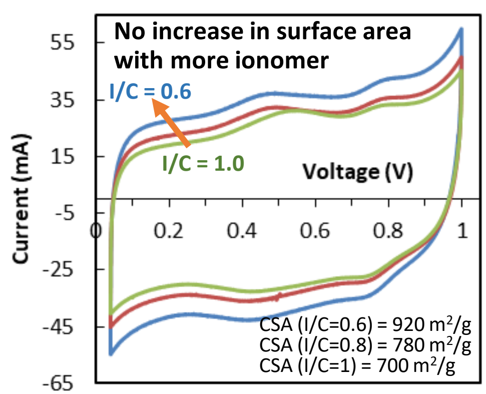
- Challenge in achieving RDE activity in MEAs due to restricted ionomer infiltration into catalyst mesopores by size exclusion.
- Nano-CT and fluorine mapping show ionomer films accumulate outside of catalyst aggregates and the interior of large particles are devoid of ionomer. Increasing the I/C ratio does not increase the CSA and worsens flooding.
- Sensitivity of CSA to RH indicates the CSA measured is partially accessed by adsorbed and condensed water domains.
- Significant opportunities for increased apparent activity with better ionomer infiltration into catalyst aggregates.

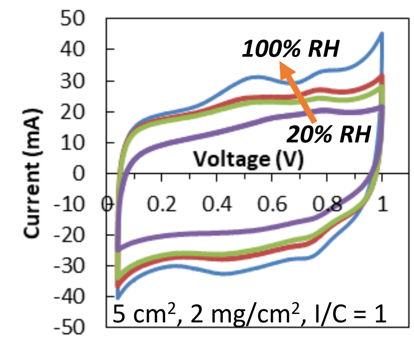


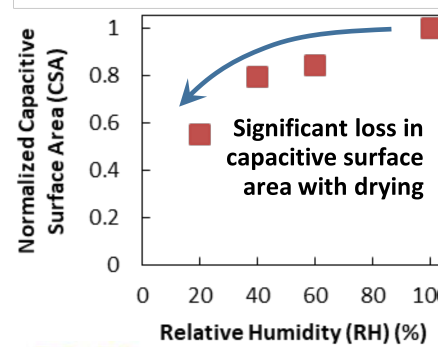


OAK RIDGE National Laboratory









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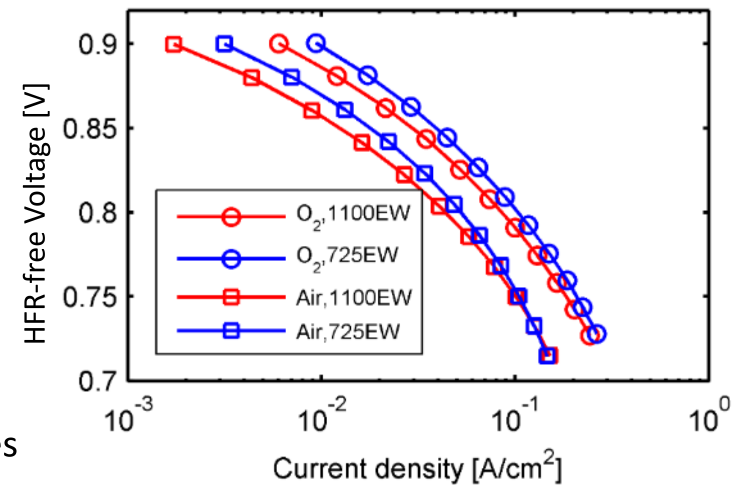
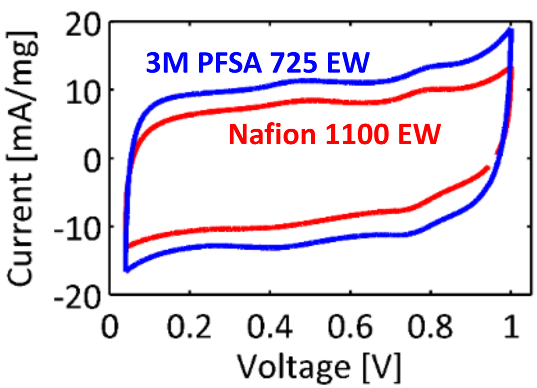
Increased Activity with Low EW PFSA Ionomer

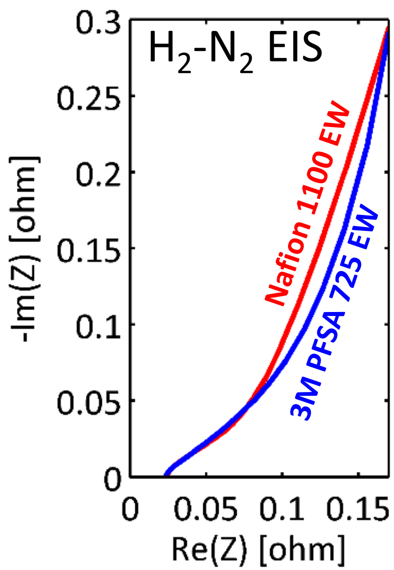
- Use of low 3M EW PSFA ionomer
- Comparison of 725 EW vs. 1100 EW Nafion
- Preliminary test with I/C = 0.6
- Significant increase in surface area and activity
- No increase in effective electrode conductivity in electrochemical impedance spectroscopy (EIS) analysis
- Indicates improved ionomer infiltration into catalyst mesopores that offsets higher conductivity of ionomer at I/C = 0.6

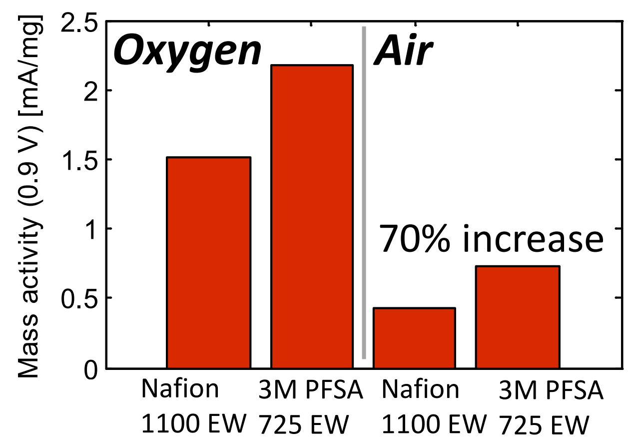
Cell temperature: 80°C; Flow rate H_2/air or O_2 :200/200 sccm
RH: 100%, 1 bar H_2/air or O_2 partial pressure. Nafion 212





CSA(1100 EW) = 450 m^2/g
CSA(725 EW) = 640 m^2/g



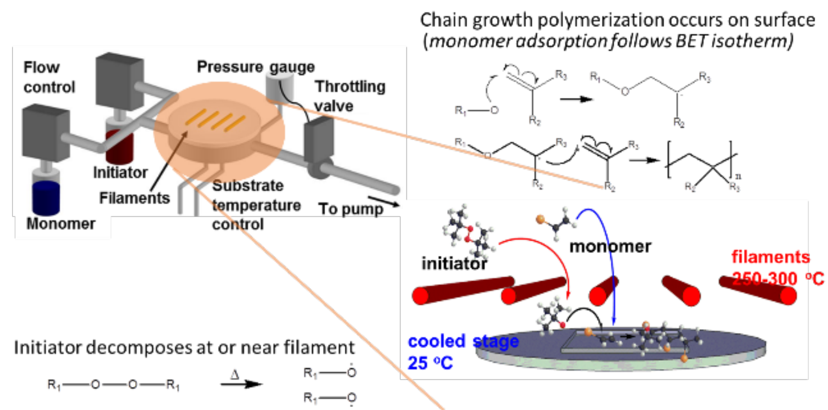


Engineered Cathode Water Management

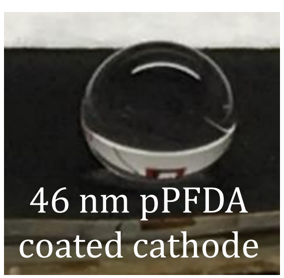
Developing multiple approaches to engineering hydrophobicity and mixed wettability to manage liquid water and O_2 diffusion, including hydrophobic support layers and hydrophobic coatings

Initiated Chemical Vapor Deposition (iCVD) of polyperfluorodecyl acrylate (pPFDA) nano-films for hydrophobicity

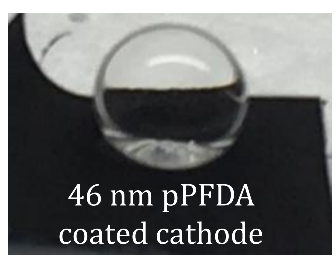
- Conformal coating of hydrophobic films down to 15 nm thickness to treat large mesopores and macropores
- Demonstrated hydrophobic coating of PGM-free cathodes
- Hydrophobicity maintained after soaking in water
- Problem: Melting point ca. 70 °C
- Solution: Co-polymerization with divinyl benzene p(PFDA-co-DVB) prevents melting below 100°C and maintains hydrophobicity



Mao, Y. et al. *Langmuir* **2004,** *20*, 2484

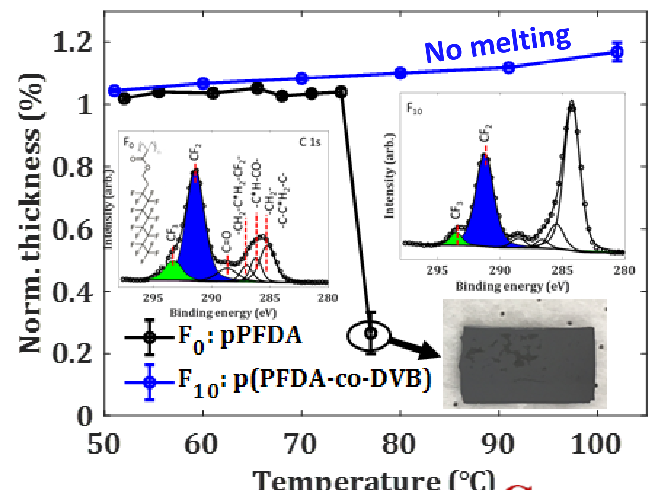


Soaking in DI water for 30 mins



Remains hydrophobic

Melting analysis by ellipsometry



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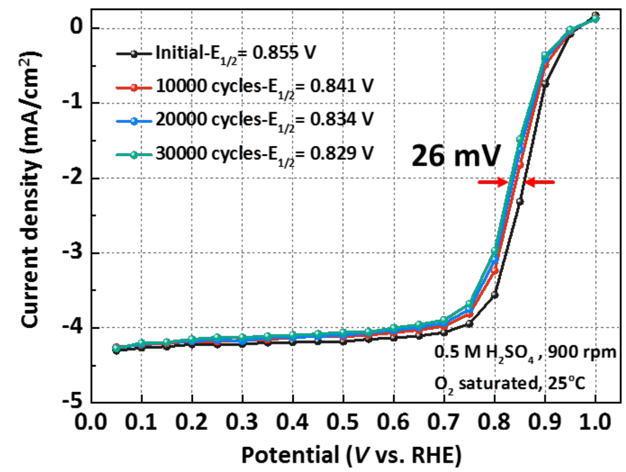
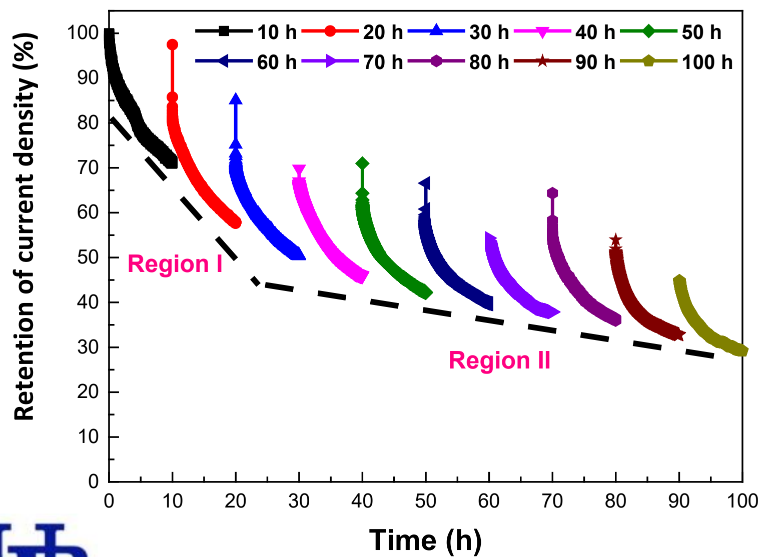
RDE Stability Studies

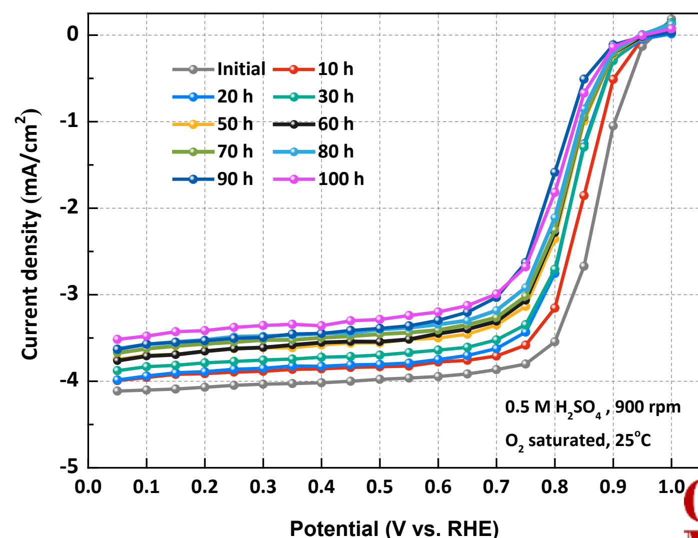
- The loss of half-wave potential is 26 mV after 30,000 potential cycles (0.6 to 1.0 V), approaching the first year's milestone ($\Delta E_{½}$ < 20 mV after 30,000 potential cycling).
- More harsh stability test conditions were developed by holding at a high potential of 0.85 V (pure kinetic region) for up to 100 hours, showing larger activity loss relative to potential cycling protocols.
- Activity loss can be divided into two regions with different degradation rates, suggesting multiple degradation mechanisms.
- Stability enhancement at high potentials will be one of future focuses by increasing carbon corrosion resistance.

Potential cycling **0.6-1.0 V** in O_2 saturated 0.5 M H_2SO_4, 25°C



Holding at a constant potential at **0.85 V** for 100 hours in O_2 saturated 0.5 M H_2SO_4, 25°C





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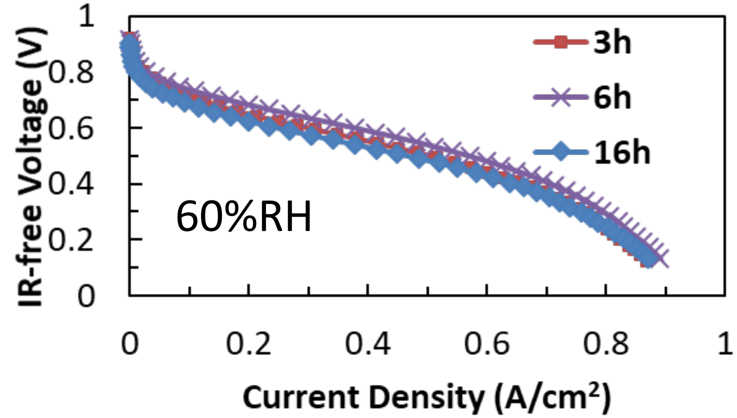
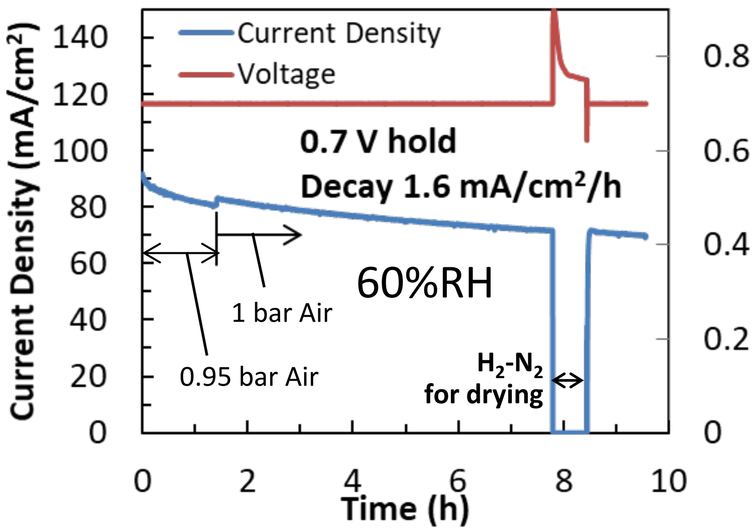
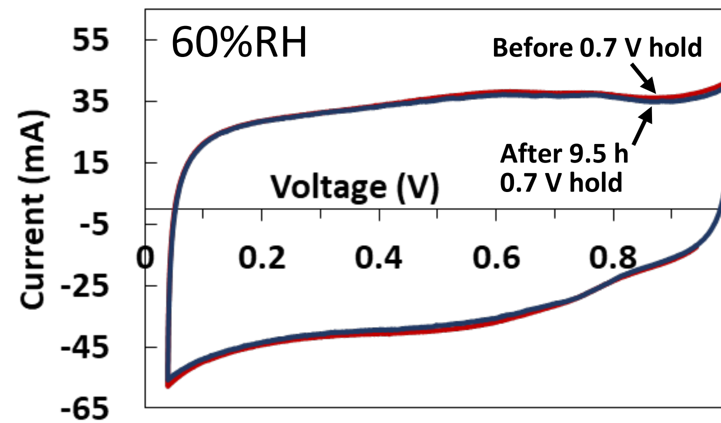
MEA Durability

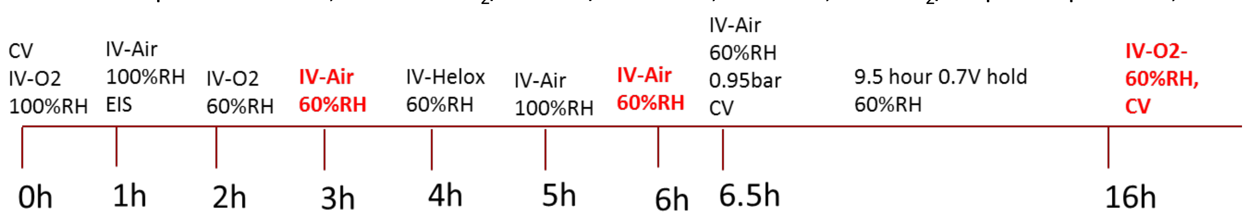
- Preliminary durability testing of MeOH solvent synthesized Fe-doped MOF catalyst at 60%
- 50 μm thick cathode (2 mg/cm^2) with I/C = 0.6
- Performance decay rate 1.6 mA/cm^2/h at 0.7 V
- Drying test at 8 h showed degradation not flooding
- No change in capacitive surface area







Cell temperature: 80°C; Flow rate H_2/Air:200/200 sccm, RH :60%, 1 bar H_2/air partial pressure, Nafion 212



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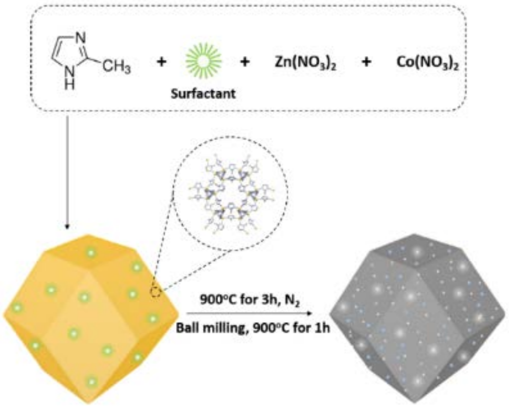
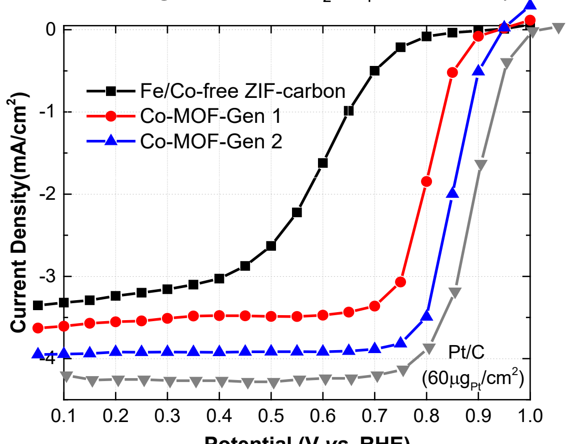
PGM-free & Fe-free Catalysts

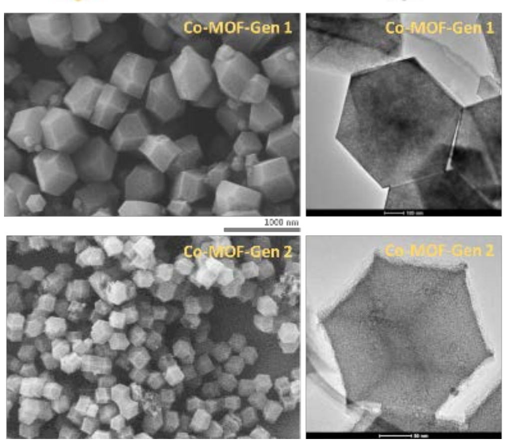
- Atomically dispersed and nitrogen coordinated **Co site catalysts** with high activity ($E_{1/2}$ = 0.85 V) at a high catalyst loading
- Remove Fe to prevent possible long-term polymer electrolyte degradation due to radical production by Fenton reaction (Fe^{2+}+H_2O_2)

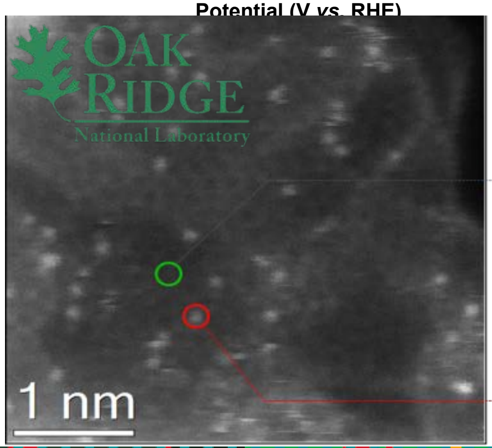
Innovative synthesis

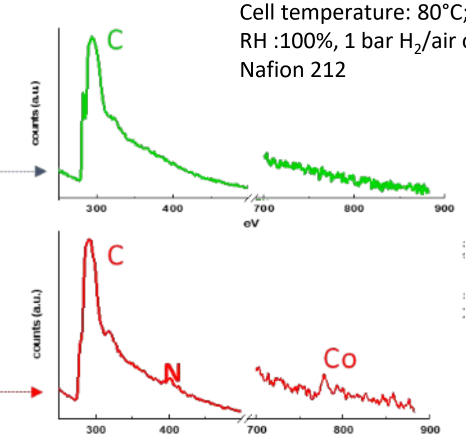


RDE: 0.8 mg/cm^2, 0.5M H_2SO_4, 25C, 900 rpm

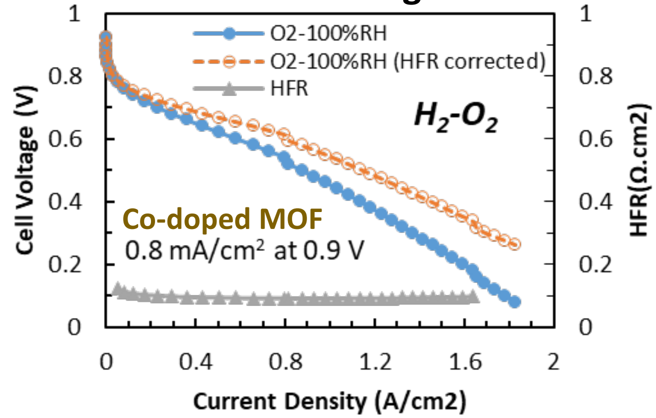


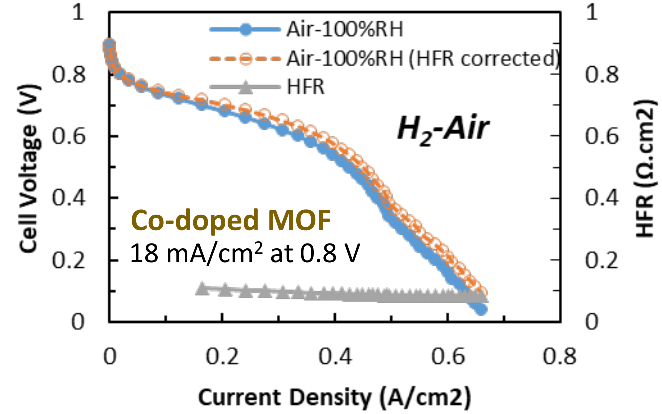






MEA Testing





Cell temperature: 80°C; Flow rate H_2/Air or O_2:200/200 sccm, RH :100%, 1 bar H_2/air or O_2 partial pressure. 4 mg/cm^2, I/C = 0.6, Nafion 212

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Technical Accomplishment

Catalyst Synthesis Scale-Up

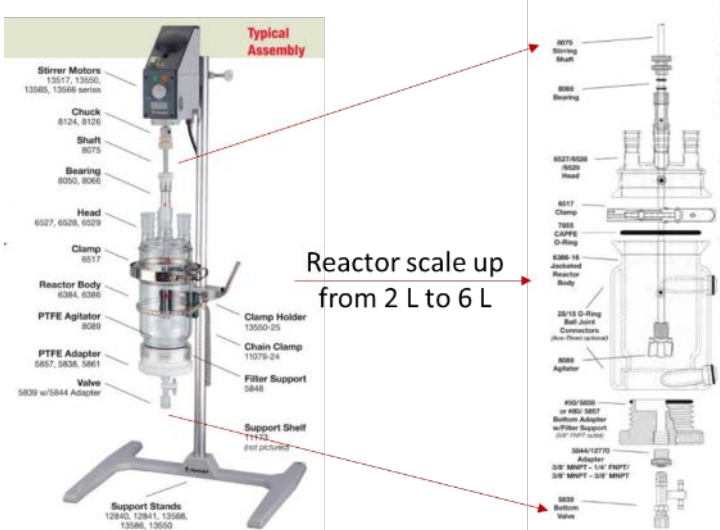
- Large amounts of down-selected catalyst with reproducible properties required for electrode optimization studies
- Scale-up of catalyst synthesis and MEA fabrication at Giner
- Initial process development and validation in 2 g batches
- Scale-up to >10 g batches

Validate the Procedure for 2 g of Fe-MOF Catalyst

Reactor validation
- Mixing zinc/iron nitrate, and 2-methylimidazolenitrate in methanol, 60°C for 24 h
- Filtering and washing with ethanol three times
- Drying precipitant at 60 °C in a vacuum oven for 12 h.
- Heating Fe-ZIF at 1100 °C under N_2 flow for 1 h

Parameter optimization
- Oil bath temperature and reacting time
- Filter disc down-selection: material, porosity, layers
- W/wo stirring vs. nucleation
- Reactant concentration vs. particle size/activity

Product validation
- Physical characterizations
- Rotating disc electrode validation
- MEA validation



Reactor scale up from 2 L to 6 L

Validate the Procedure for > 10 g of Fe-MOF Catalyst

Procedure optimization
- Reactant concentration optimization
- Mixing process control
- Oil bath temperature and reacting time

Product validation
- Rotating disc electrode validation
- Rotating disc electrode validation
- Physical characterizations

Reponses to Last Year AMR Reviewers' Comments

- New project - not reviewed in 2017

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Future Work

- **Improving durability** by tuning synthesis and resulting carbon structure for greater carbon oxidation resistance and metal-atom retention
- **Improving the understanding of the active site** through DFT modeling and molecular probes studies with Los Alamos and other ElectroCat consortium members
- **Increasing mass activity** by adjusting MOF-derived catalyst aggregate diameter and primary pore size for improved ionomer integration
- **Increasing power density** by mitigating flooding by implementing p(PFDA-co-DVB) coating in operating fuel cells and introducing hydrophobic support layers
- **Reducing voltage losses** by optimizing catalyst ink composition and processing, including ionomer loading and EW
- **Increasing catalyst supply rate** by scaling up synthesis of down-selected catalysts
- **Streamlining MEA production** by establishing improved cathode ink deposition methods for catalyst coated membranes (CCMs) and gas diffusion electrodes (GDEs)

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

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Summary

Approach

An integrated approach to achieving PGM-free cathodes with high power density and durability through three key approaches utilizing the strengths of the project team:

1. **Advanced MOF-derived M-N-C catalysts** with a high activity and durability. Features a low cost synthesis of atomically dispersed active sites at high spatial density
2. **PGM-free specific cathode architectures** that address the substantial flooding and transport resistances in thicker catalyst layers by introducing engineered hydrophobicity through additives and support layers
3. **Advanced ionomers** with low EW for increased activity and offering high proton conductivity for low ohmic losses across the electrode and more uniform catalyst utilization for improved durability

Accomplishments and Progress in First Seven Months

- Atomically dispersed catalyst using Fe- and Co-doped MOF have demonstrated high activity, including those with precursors synthesized with a green H_2O solvent
- Established an understanding of aggregate and primary particle size effect on MEA performance
- Identified enhanced performance with low EW ionomers
- Development of novel thin-film hydrophobic iCVD coatings for introducing hydrophobicity
- MEA and DFT models established to guide cathode and active-site engineering

Collaboration and Coordination with Other Institutions

- Rapid iteration cycle with catalyst development at UB and MEA fabrication and testing at CMU.
- Catalyst scale-up at Giner using UB developed process
- Ionomer integration at CMU using 3M ionomer
- ElectroCat consortium actively collaborating on XAS, XRF, electron microscopy, and electrode fabrication

Relevance/Potential Impact

- Advancing synthesis of atomically dispersed active sites at high density with a simplified, low cost approach in order to meet activity and stability targets.
- Establishing new cathode designs specifically for PGM-free catalysts such that active sites are efficiently utilized to enable high power densities with durable performance.

Proposed Future Work

- Improving stability with more durable carbon phases
- Improving the understanding of the active site through DFT and advanced analytical methods
- Increasing mass activity through morphology and active site density
- Increasing power density with engineered water management
- Reducing Ohmic voltage losses with improved ionomers
- Increasing catalyst supply rate through scale-up
- Streamlining MEA production with standardized fabrication methods

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Acknowledgements

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Hoon Chung
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Sunilkumar Khandavalli
Scott Mauger

Oak Ridge National Laboratory
Karren More
David Cullen

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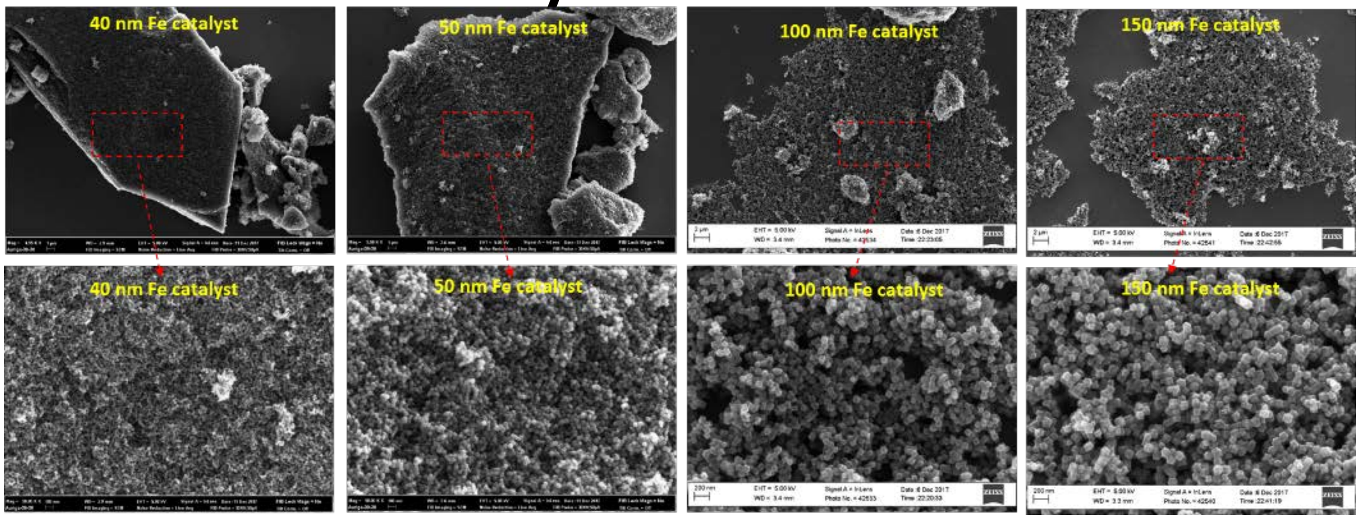
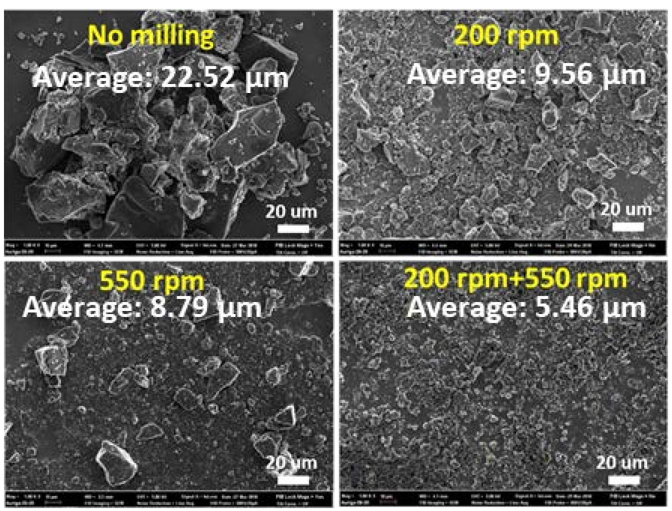
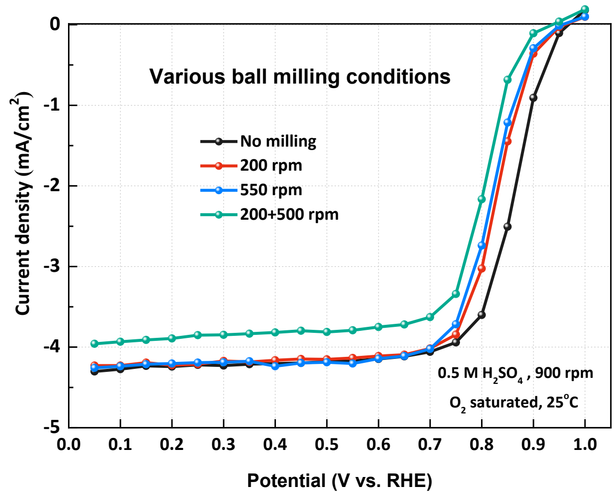
Technical Backup Slides

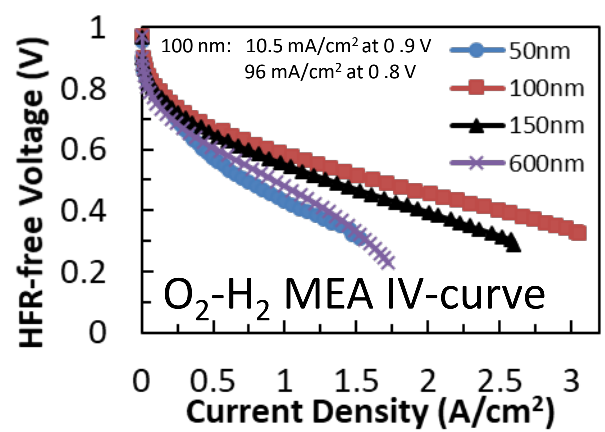
Engineering Morphology by Controlling Primary and Secondary Particle Sizes



- Catalysts polyhedron particles with smaller size shows better performance in RDE
- Smaller size, more significant agglomeration forming dense and large secondary particles up to 20-30 µm
- Such agglomeration is not favorable for fuel cell performance
- Ball milling process is able to reduce the sizes of aggregates, but leading to reduced RDE activity







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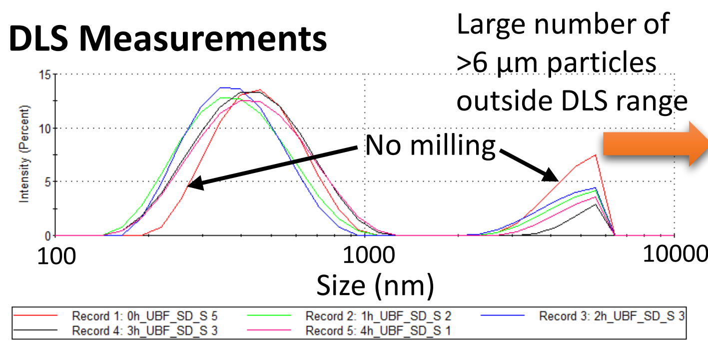
MEA catalyst loading: 4 mg/cm², Cell temperature: 80°C; Flow rate H_2/O_2 :200/200 sccm
RH: 100%, 1 bar H_2/O_2 partial pressure. Nafion 212

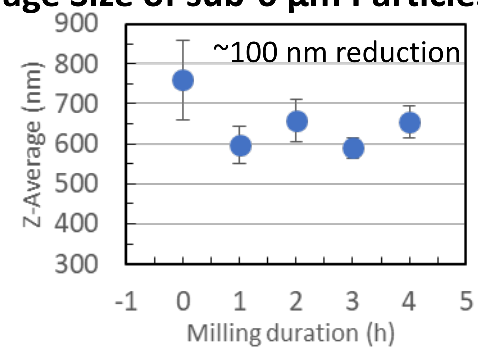
NREL Particle Size and MEA Fabrication

- MEA fabrication process studies and alternative MEA fabrication strategies at NREL
- Dynamic light scattering (DLS) measurements of particle size as function of ball milling time
- Only minor size reduction by ball milling and significant portion of volume and active sites in large particles
- Preliminary reaction kinetics study by polarization curves at varying O_2 partial pressure and cell temperature for inputs for MEA model's reaction kinetics

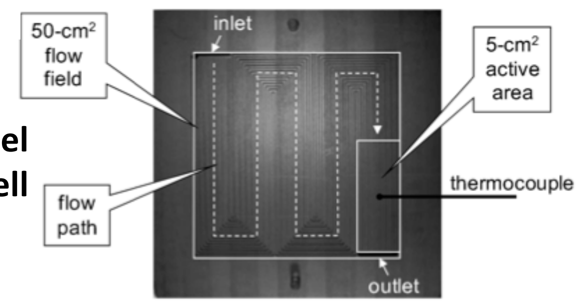
DLS Measurements

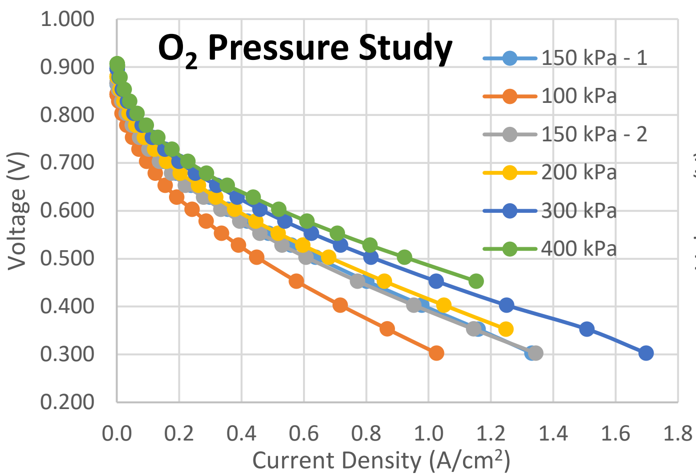


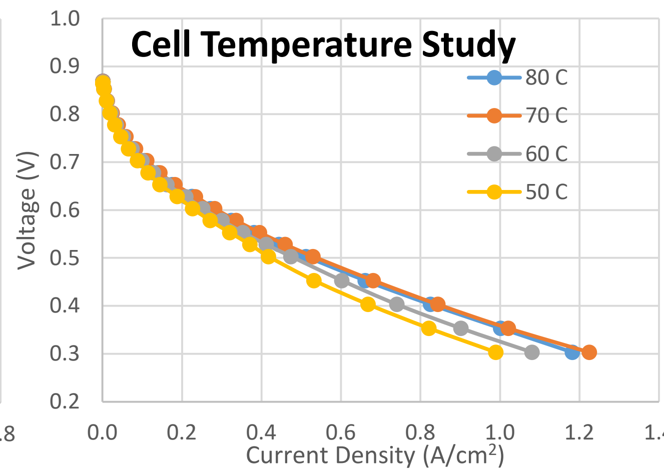
Average Size of sub-6 µm Particles



NREL parallel channel differential cell







NREL NATIONAL RENEWABLE ENERGY LABORATORY

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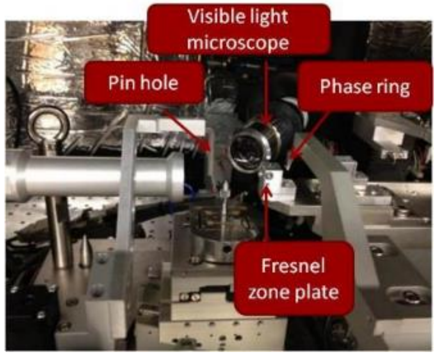
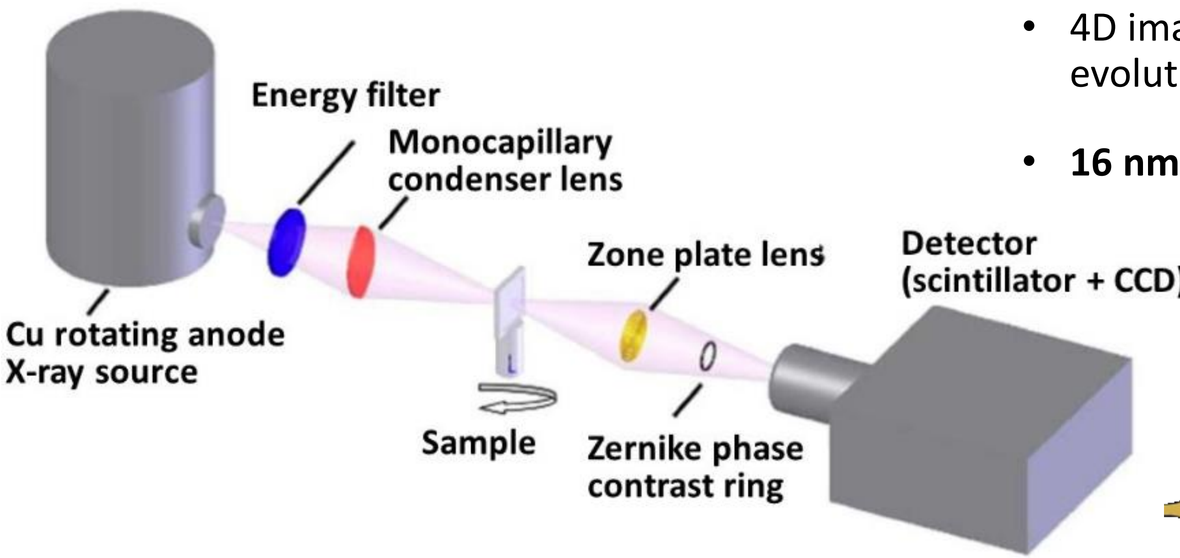
Cell temperature: 80°C; Flow rate H_2/ O_2 :300/300 sccm
RH: 100%, 1 bar H_2/air or O_2 partial pressure. Nafion 211

Nano-CT at CMU



User Facility: www.cmu.edu/me/xctf



- User facility with internal and external users. Primary use in electrochemical energy materials
- Xradia UltraXRM-L200 Nano-CT
- Laboratory 8 keV Cu rotating anode X-ray source
- Non-destructive imaging in ambient and controlled environments
- 4D imaging (space and time) for material evolution studies
- **16 nm voxels, 50 nm resolution**

NSF MRI award 1229090
(PI: Litster; Co-PIs: De Graef, Fedder, Feinberg, Sullivan)

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New Microstructure Model Framework for Large Scale Simulation

- Reimplementation of prior cathode microstructure model
- Open-source MOOSE finite element package from Idaho National Lab
- Highly parallelizable for multiphysics simulation over large domains
- Simulation on Amazon AWS instance (64 cores, 488 GB RAM)
- 30-40 µm size domains resolved with high resolution features
- 30-60 min per condition with ~20M elements
- Captures heterogeneity in transport properties and ORR current density

LANL CM-PANI-Fe Cathodes