ElectroCat: PGM-free Engineered Framework Nano-Structure Catalysts

2018 DOE Hydrogen and Fuel Cells Program Review Presentation

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Project ID # FC173

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Overview

Timeline

- Project start date – 09/01/2017
- Project end date – 08/31/2020
- Percent complete – 19.6%

Barriers

- A. Durability (Catalyst)
- B. Cost (Catalyst)
- C. Performance (Catalyst, MEA)

Budget

- Total project funding
  - $2,000,000 (DOE share)
  - $500,000 (Cost share)

Partners

- Greenway Energy, LLC (Project Lead)
- Savannah River National Laboratory (Subcontractor)
- Northwestern University (Subcontractor)
- Ballard Power Systems (No Cost Partner)
- Los Alamos National Laboratory (Core Lab)
- Oak Ridge National Laboratory (Core Lab)

Relevance

Overall Objective: Develop durable, highly active electrocatalysts for the ORR through a unique, bottom-up, rational design that will enable a better understanding of the PGM-free active site and improve activity.

- This project addresses technical targets from DOE's FCTO Multi-Year R&D Plan to enable commercialization of fuel cell electric vehicles by improving the performance and durability, while reducing the cost of PGM-free catalysts.

FY2018 Objectives: High throughput catalyst development targeting porphyrinic and "phen" type active sites; explore heteroatom doping; begin in house MEA optimization and FC testing; align core lab ORR active site modeling with experimental approach.

Metric	Units	FY18 Target	FY19 Target	FY20 Target	2020 DOE Target
Fuel Cell test: Catalyst Activity	mA cm^{-2} @ 900 $mV_{IR\text{-}free}$	≥ 20[b]	≥ 25[b]	≥ 30[b]	≥ 44[a]
Fuel Cell test: Catalyst Activity	mA cm^{-2} @ 800 mV	NA	NA	≥ 150[c]	NA
RRDE test: Catalyst Activity	mA cm^{-2} @ 800 mV	≥ 1.5[d]	≥ 2.0[d]	NA	NA

[a] 80°C H_2/O_2 MEA; fully humidified, total outlet pressure 150 kPa; anode stoich 2; cathode stoich 9.5
[b] 80°C H_2/O_2 in an MEA; total outlet pressure of 100 kPa
[c] 80°C H_2/Air in an MEA; total outlet pressure of 100 kPa
[d] 0.1 M $HClO_4$ acid; catalyst loading of 0.6 mg cm^{-2}

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Approach

Bottom-up, rational synthesis plan designed to incorporate known functionalities into high surface area microporous frameworks.

Unique Design Features

- Frameworks can be engineered to have high activity for the ORR by
  - maximizing the number of accessible active sites through integration of functional groups into the polymer skeleton
  - maximizing surface area (BETs up to 3000 m^2/g)
  - tailoring pore size to optimize catalyst/ionomer interface (improved ORR kinetics)
- Inherent chemical and thermal stability (catalysts can be designed to endure accelerated stress protocols)
- Low-cost manufacturing
  - low cost precursor chemicals
  - low number of syntheses and/or processing steps

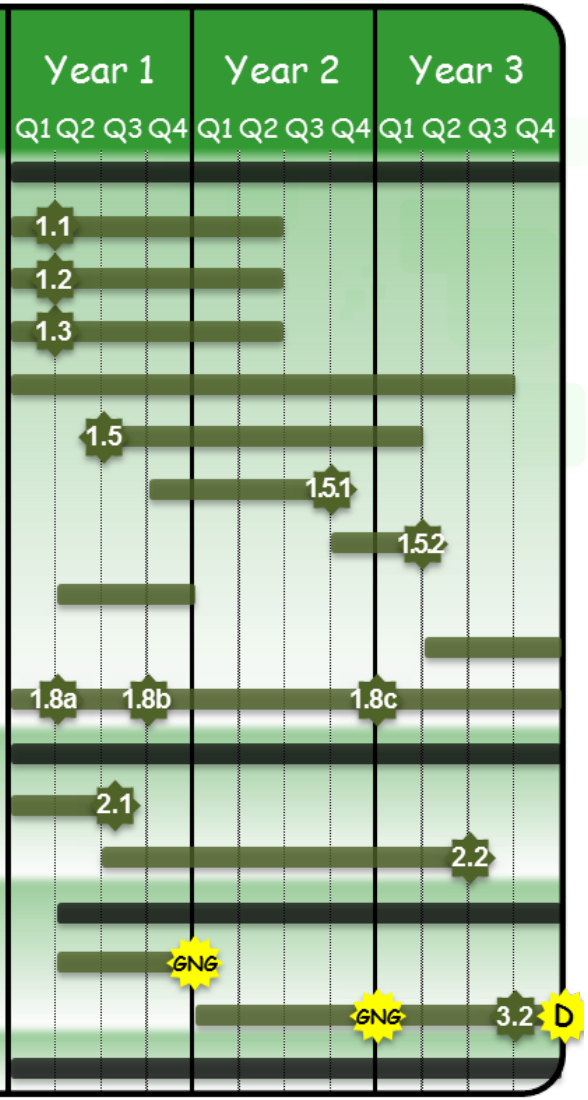
Approach

Current Focus
Screened >12 material families

Task Initiated

Core Lab Focus (LANL)

Task	Program Activities
1	**Catalyst development based on high surface area polymers**
1.1	Synthesize "phen" type chelating polymers
1.2	Synthesize porphyrinic polymers
1.3	Synthesize high N carbon based catalysts
1.4	Post synthesis treatment of catalysts materials
1.5	High throughput synthesis of engineered frameworks
1.5.1	Improve catalyst performance through heteroatom addition
1.5.2	Improve catalyst performance by adding peripheral functionalities
1.6	Synthesize catalysts and fabricate MEA for interim fuel cell test
1.7	Synthesize catalysts and fabricate MEA for final fuel cell test
1.8	Electrochemical and Physical Characterizations
2	**Active Site Modeling**
2.1	Align core lab modeling with experimental results
2.2	Model proposed structures using experimental results
3	**MEA Optimization and Fuel Cell Testing**
3.1	Initial MEA optimization studies
3.2	MEA optimization studies with optimized catalysts
4	**Program Management and Technology Transfer Strategy**



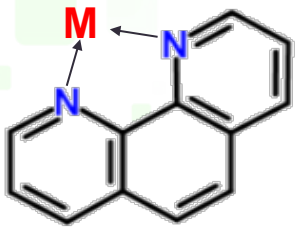
Approach

Milestone	Year 1 Project Milestones	Type	Scheduled Completion (Quarter)	Percent Complete	Progress Notes
1.1	Optimize synthesis protocol to prepare >400 mg of “phen” type chelating polymers per batch	Milestone	Q1	100%	Complete
1.2	Optimize synthesis protocol to prepare >400 mg of porphyrinic polymers per batch	Milestone	Q1	100%	Complete
1.3	Optimize synthesis protocol to prepare >400 mg of high N containing carbon based materials per batch	Milestone	Q1	100%	Complete
1.5	Down select polymeric materials for high throughput synthesis	Milestone	Q2	33%	In progress
1.8a	Demonstrate improved ORR activity through transition metal coordination.	Milestone	Q1	100%	Complete
1.8b	RRDE performance >1.5 mA cm^{-2} at 0.8 V vs. RHE	Milestone	Q3	100%	Complete
2.1	Align core lab modeling with experimental approach	Milestone	Q2	100%	Complete
GNG	Demonstrate H_2-O_2 fuel cell performance that meets or exceeds 20 mA cm^{-2} at 0.90 $V_{IR\text{-}free}$	Go/No-Go	Q4	10%	In progress

Accomplishments and Progress

Task 1.1: "phen" type chelating Frameworks

Overview

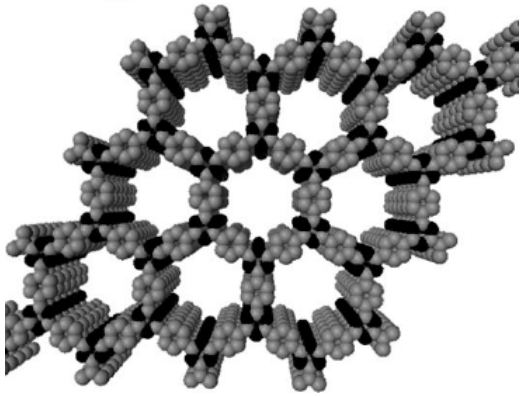


MN_2C_y

"phen" type chelating frameworks

- MN_2C_y type carbon catalyst structure
- bidentate, chelating ligands such as 1,10-phenanthronline, 2,2'-bipyridine and their derivations

Focus Area #1



CTF-1

Covalent Triazine Framework (CTF)

- micro/mesoporous semi-crystalline high surface area polymer
- organic linker influences properties (pore-size, chelating sites, conductivity)
- <u>active sites must be incorporated</u> into the linker to impart catalytic activity for the ORR

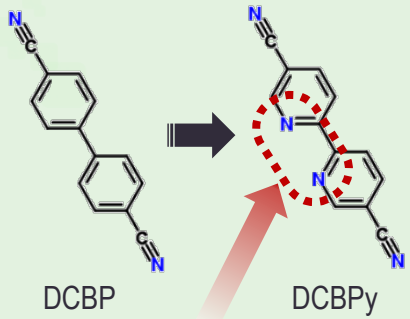
Accomplishments and Progress

Task 1.1: "phen" type chelating Frameworks

Focus Area #1 – Covalent Triazine Frameworks

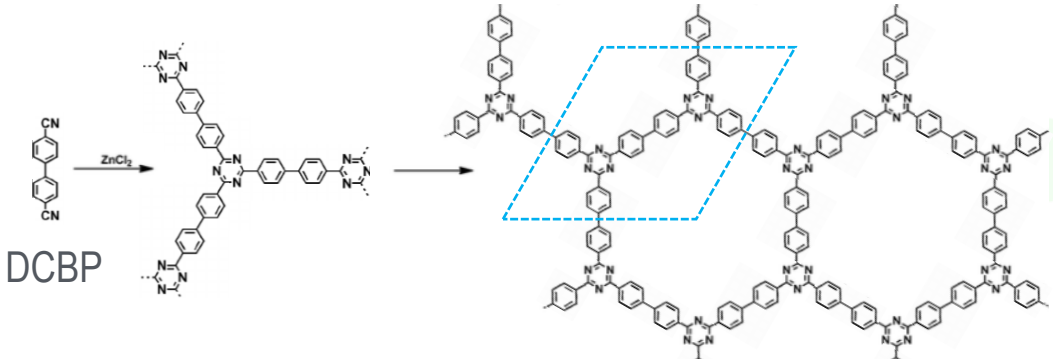
- single-step self-assembly of 3D frameworks
- active sites must be incorporated into the linker to impart catalytic activity for the ORR

CTFs based on DCBP and DCBPy

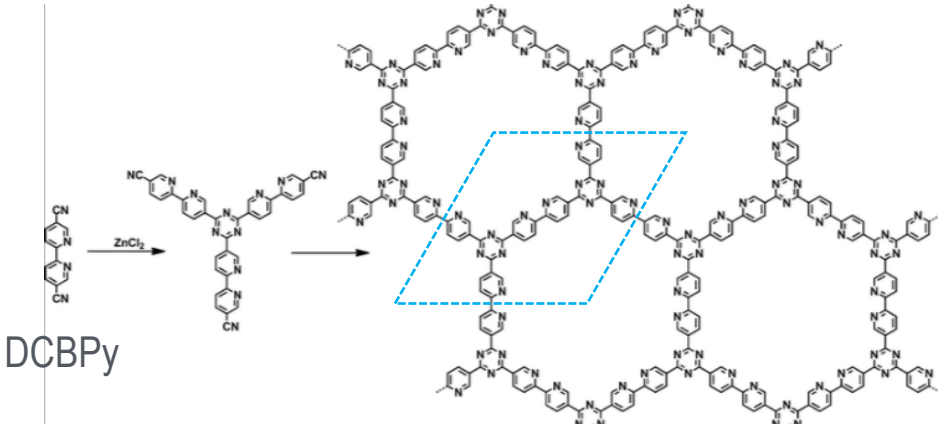


Incorporate chelating sites within monomer

CTF based on 4,4'-dicyanobiphenyl (DCBP)



CTF based on 5,5'-dicyano-2,2'-bipyridine (DCBPy)

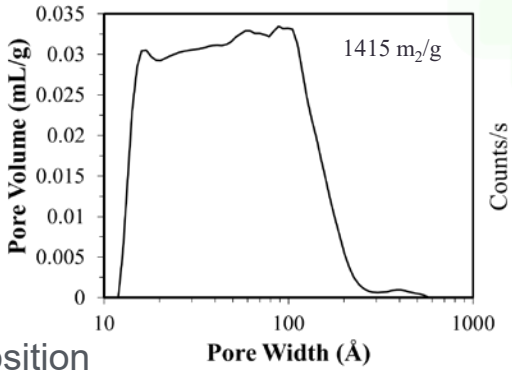


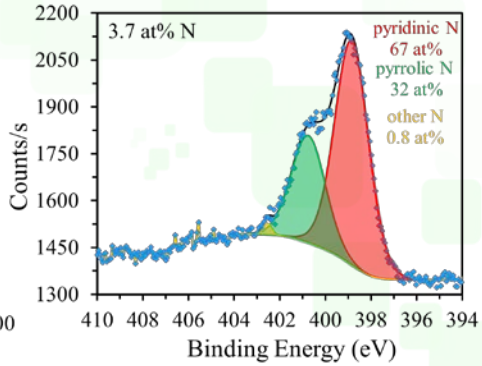
Accomplishments and Progress

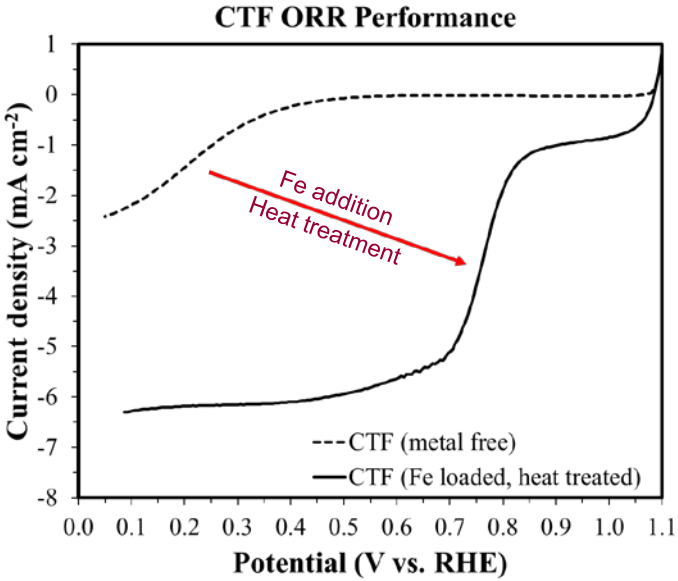
Task 1.1: "phen" type chelating Frameworks

Focus Area #1 – Covalent Triazine Frameworks

- CTF polymers based on DCBP and DCBPy with "phen" type chelating sites have been synthesized
- Metalation and post-synthesis treatments of CTFs under development, optimizing procedures
  - Metal loading
  - Loading time
  - Pyrolysis temperature, duration, and gas composition
- Electrochemical Characterization
  - Metal free CTF is electrically conductive without heat treatment and shows ORR at low potentials
  - Fe addition + heat treatment shows increase in ORR activity







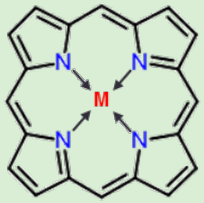
Highlights

- BET analysis shows surface area of 1415 m^2/g and pore volume of 1.32 mL/g (large mesopore volume)
- XPS analysis of CTF with 9:1 DCBP/DCBPy shows N content of 3.7 at% with a high ratio of pyridinic/pyrrolic N
- Metalation protocol requires optimization, does not currently meet electrochemical performance targets

Accomplishments and Progress

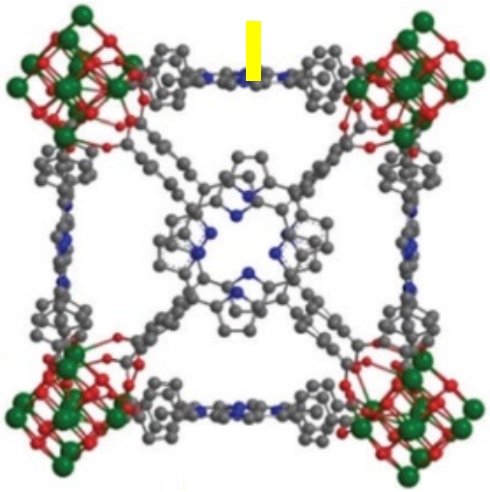
Task 1.2: Porphyrin Containing Frameworks

Overview



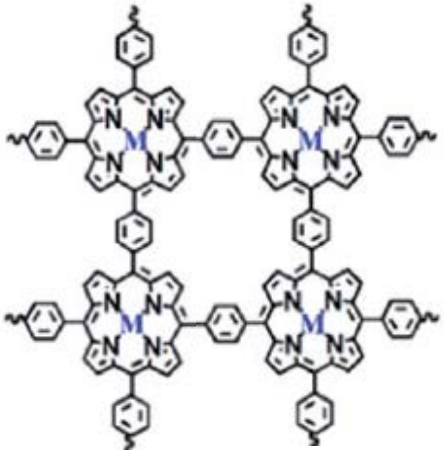
- Porphyrin containing frameworks
  - FeN_4 type carbon catalyst
  - includes porphyrins, phthalocyanines and other macrocycles

Focus Area #1



Porphyrinic MOF based materials

Focus Area #2

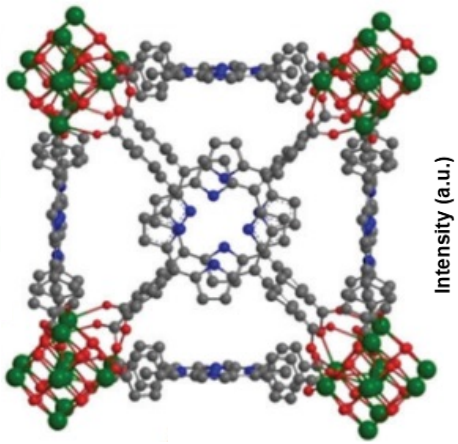


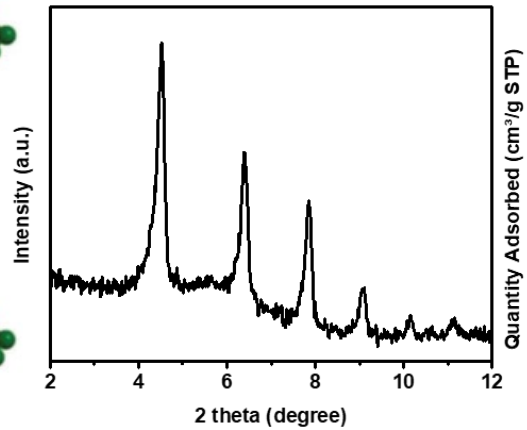
Polyporphyrin based materials

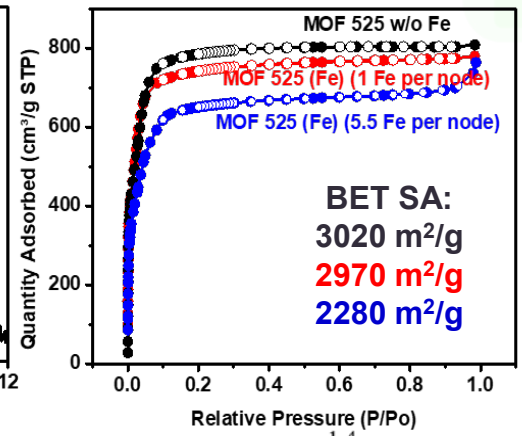
Accomplishments and Progress

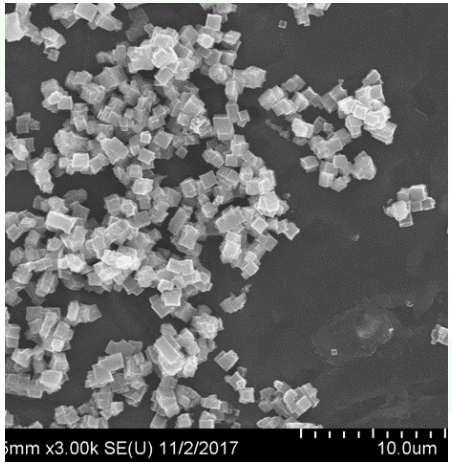
Task 1.2: Porphyrin Containing Frameworks

Focus Area #1 – MOF 525



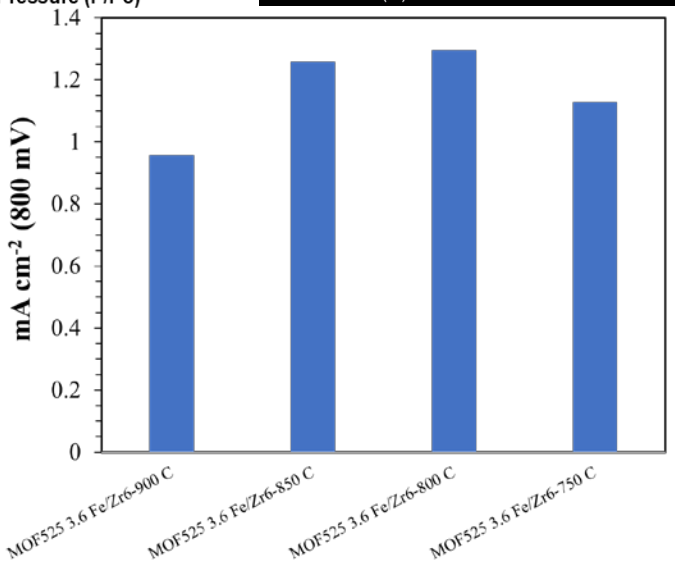






MOF 525 structure and properties

- 3D MOF with a ftw topology
- 12-connected Zr6 nodes
- 4 linker- tetracarboxyphenylporphyrin
- High stability and surface area



Highlights

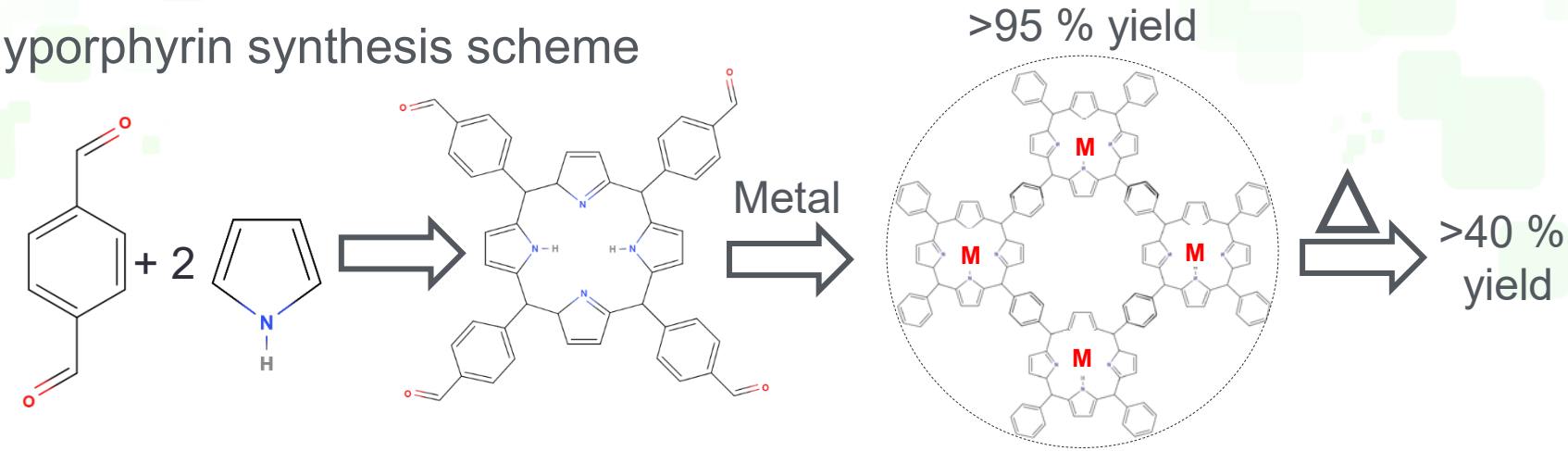
- Higher performance is obtained with a slight excess of Fe
- Optimum heat treatment temperature for ORR performance is obtained around 800 ºC
- No synergistic effect is observed from Zr in the structure

Accomplishments and Progress

Task 1.2: Porphyrin Containing Frameworks

Focus Area #2 – Polyporphyrin

Polyporphyrin synthesis scheme



- synthesis conditions have been developed and optimized to maximize catalyst performance
- 500 mg batches are routinely prepared, process is amenable to significant scale-up

Highlight

- Catalyst utilizes low cost precursors, simple scale-up, and requires little post treatment

(see preliminary cost analysis, right)

Preliminary Cost Analysis

Chemical	Cost/Synthesis	Cost/g After Heat Treatment
Pyrrole	$0.21*	~$1.05/g‡
Terephthalaldehyde	$0.15*	
Fe salt	$.00825*	

*price based on small quantity chemical lab suppliers

‡catalyst cost based only on precursor cost

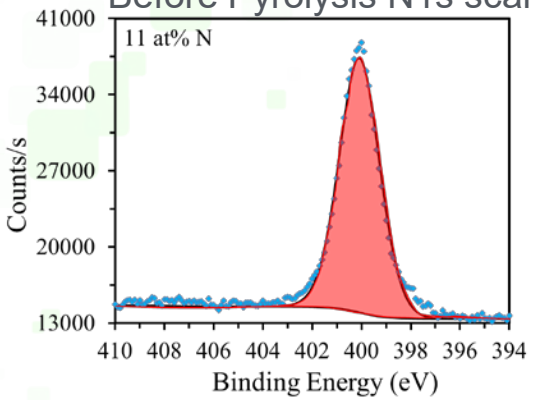
Accomplishments and Progress

Task 1.2: Porphyrin Containing Frameworks

Focus Area #2 – Polyporphyrin

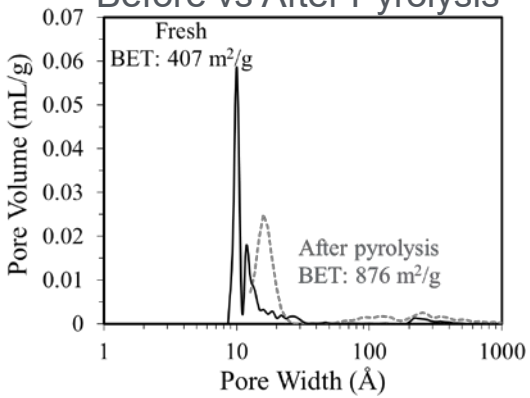
XPS

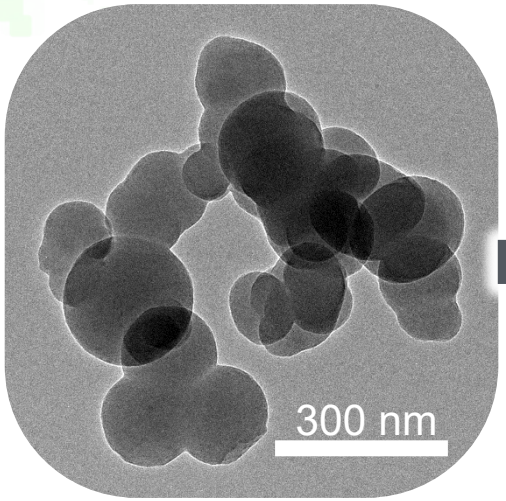
Before Pyrolysis N1s scan

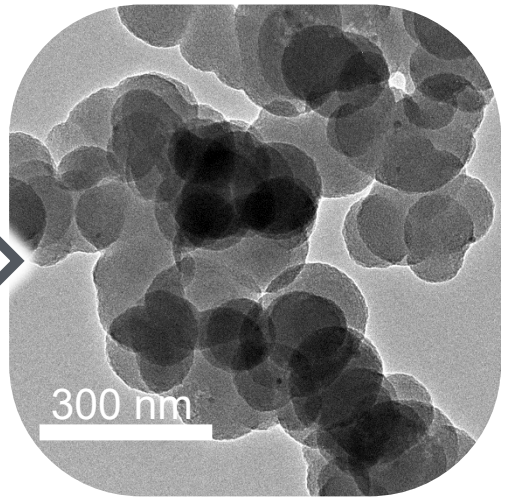


BET

Before vs After Pyrolysis







Physical Characterization

Before Pyrolysis

- XPS shows nitrogen content around 11 at%
- TEM shows particles between 100-200 nm
- BET surface area around 400 m^2/g

After pyrolysis

- TEM shows no particle size change
- TEM shows increase in surface roughness
- BET analysis shows an increase in surface area (876 m^2/g)

Highlight

- Single step reaction followed by one pyrolysis shows catalysts with promising properties

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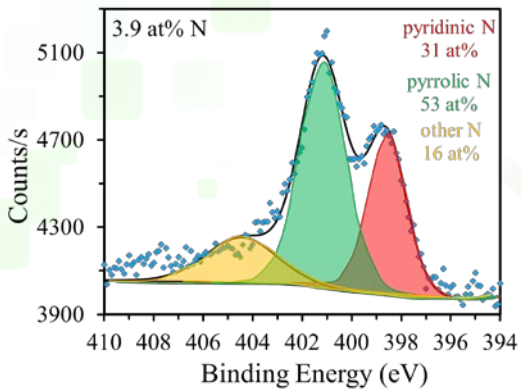
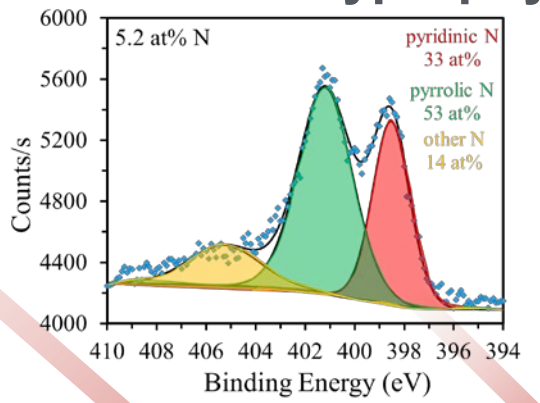
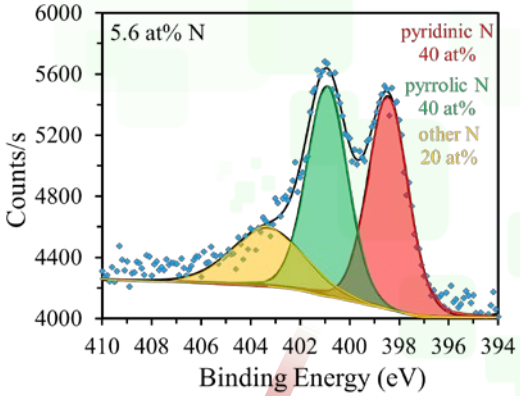
Task 1.2: Porphyrin Containing Frameworks

Focus Area #2 – Polyporphyrin





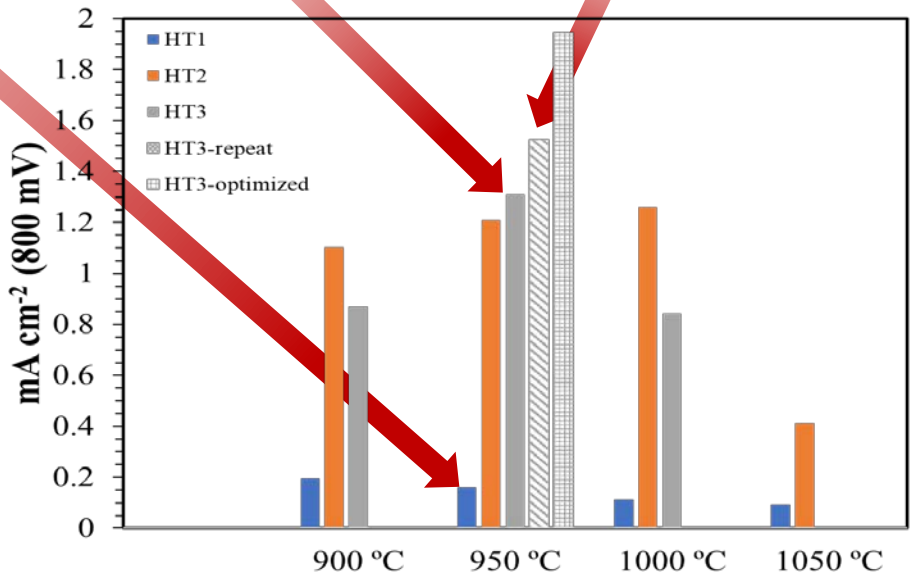


Physical Characterization

- N content and pyridinic/pyrrolic ratio can be tailored through heat treatment conditions
- XPS analysis shows N content from 4-6 at%

Electrochemical Performance

- Increasing pyridinic N correlates with increasing ORR performance



Highlight

- Catalysts based on polyporphyrins approach state of the art performance

RDE ORR performance @ 800 mV: ~2 mA/cm^2

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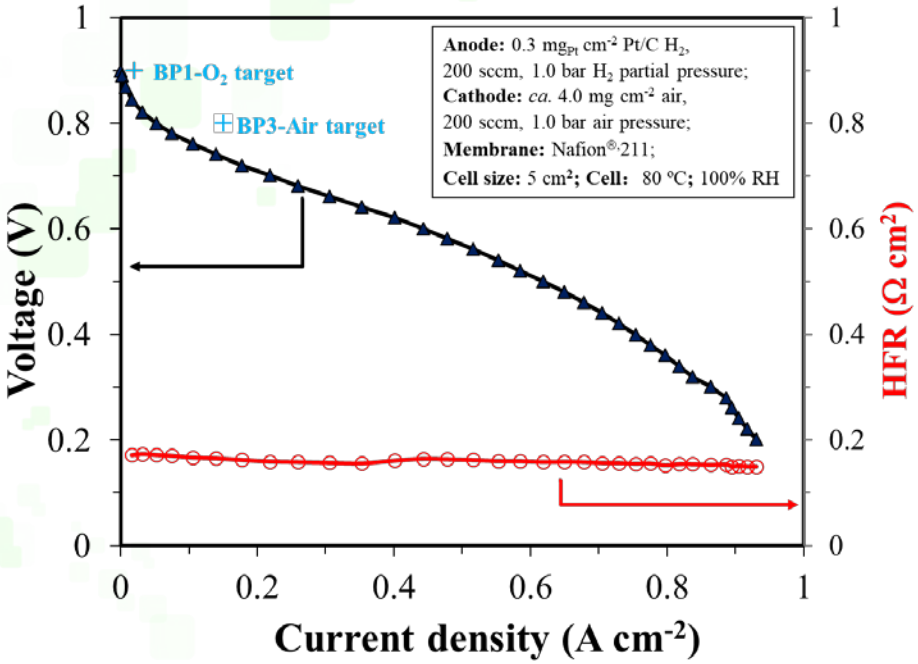
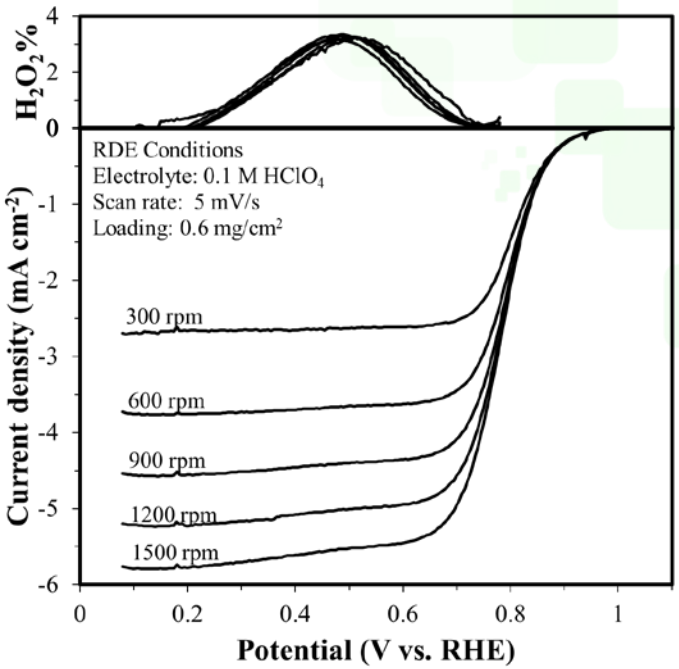
Task 1.2: Porphyrin Containing Frameworks

Focus Area #2 – Polyporphyrin





- FC performance of the un-optimized porphyrinic catalyst was evaluated at LANL
  - Initial air performance shows ~53 mA/cm^2 at 800 mV
- MEA optimization and FC performance of optimized porphyrinic catalyst is underway

RRDE evaluation of electrocatalysts shows

- < 3.4% H_2O_2 or >3.94 # e^-
- $E_{1/2}$= 0.79 V vs. RHE after cycling

Highlight

- Initial air performance shows ~53 mA/cm^2 @ 800 mV
- High selectivity towards the 4 e^- reaction

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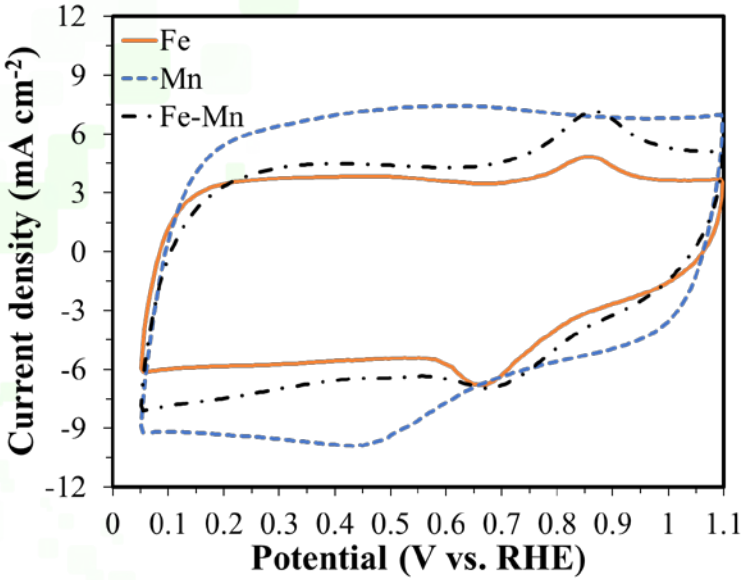
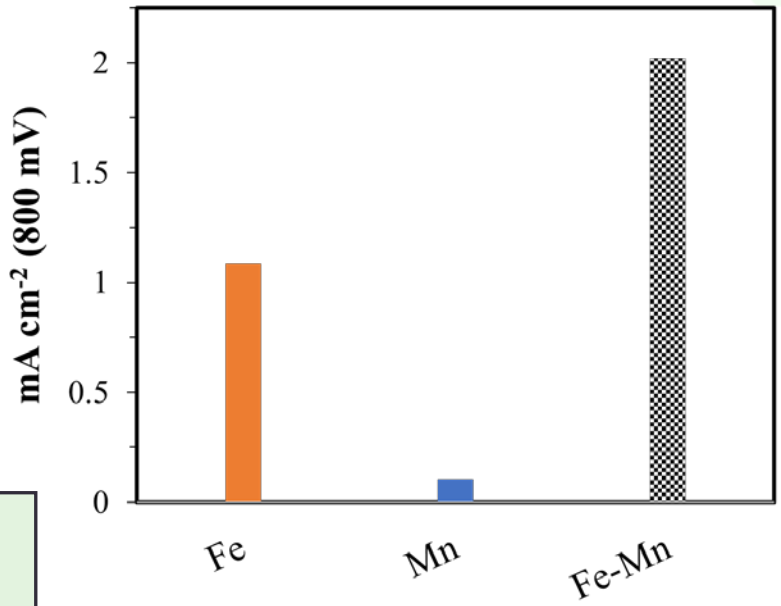
Task 1.2: Porphyrin Containing Frameworks

Focus Area #2 – Polyporphyrin



Metallated Polyporphyrins

- Use of Mn as the metal coordinated in the porphyrin ring was explored
  - Mn shows an increase in the electrochemical surface area
  - Mn shows lower activity at 800 mV
- Combination of Mn and Fe shows promising initial performance



Electrochemical Performance

- Fe-Mn coordinated porphyrin ring, shows an increase in the on-set potential
- Different strategies are being implemented to stabilize the initial performance

Highlight

- Mn only catalyst shows low activity
- As an additive, Mn improves Fe-based catalyst performance

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Accomplishments and Progress

Task 1.3: High N Carbon Based Catalysts

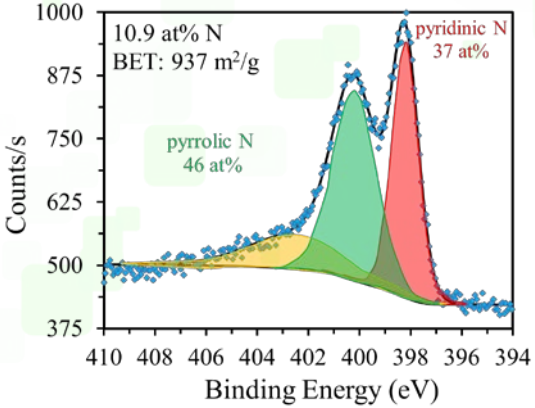
Overview

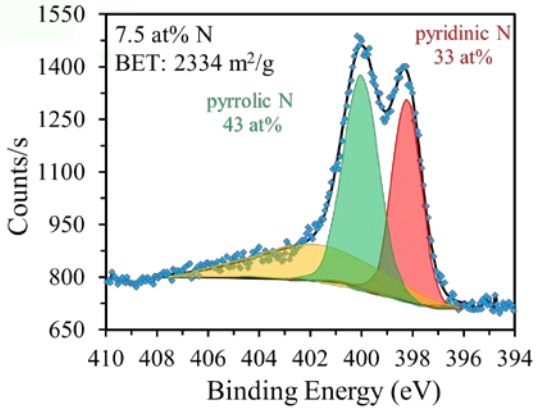
Highly scalable process has been developed to

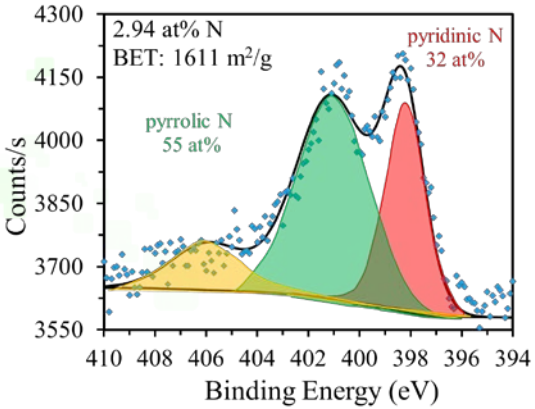
- Maximize N content
- Control pyridinic/pyrrolic N content
- Maximize surface area of carbon materials using inexpensive chemical precursors

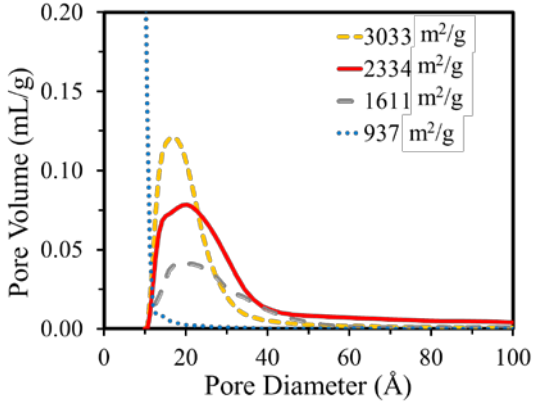
Accomplishments and Progress

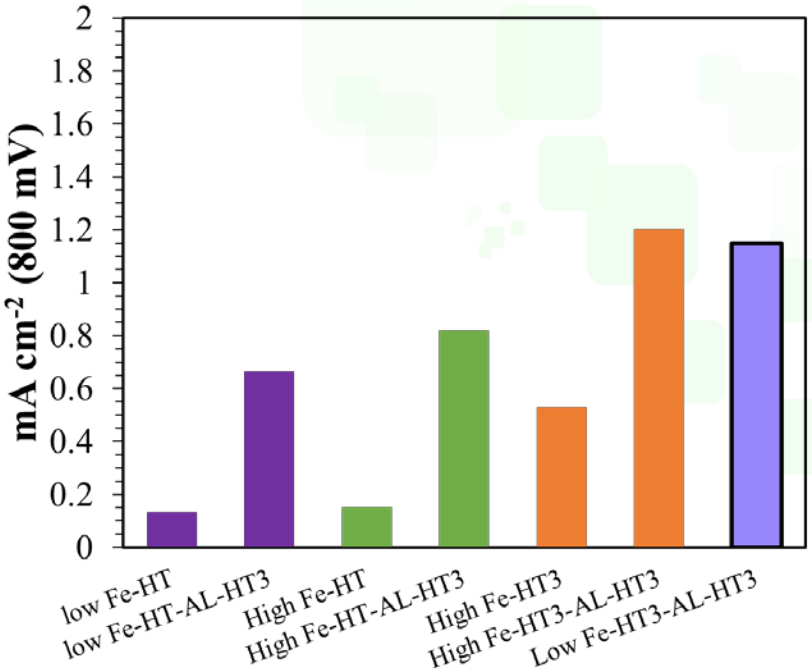
Task 1.3: High N Carbon Based Catalysts











- XPS analysis of catalyst materials show N content up to ~11 at% N
  - >30 at% pyridinic N and >40 at% pyrrolic N
- High BET surface areas (900 to 3000 m^2/g) and varied pore size distribution

Highlight

- High surface area and nitrogen content was achieved using easy to tailor highly scalable processes
- Optimization is underway to maximize ORR performance

Accomplishments and Progress

Task 2.1: Active site modeling

Overview

- Graphene Bulk and Edge Sites with substitutional sites are evaluated towards oxygen reduction to water
  - FeN_4 for Fe^{II}
  - $HOFeN_4$ for Fe^{III}
  - $OFeN_4$ for Fe^{IV}

- Predictions from DFT Models
  - linear Gibbs energy relationship (LGER) and chemical hydrogen electrode (CHE) models are being used

LGER process replaces $\Delta_{ads}G$ *with* $\Delta_{ads}E$

$$\mathbf{Ox(aq) + e^-(U^0) \rightleftharpoons Red(aq) \quad (U^0 exptl)}$$

$$\downarrow \Delta_{ads}G(Ox) \qquad \downarrow \Delta_{ads}G(Red)$$

$$\mathbf{Ox(ads) + e^-(U_{ads}) \rightleftharpoons Red(ads)}$$

$$\mathbf{U_{ads} = U^0 - \Delta_{ads}G(Red) + \Delta_{ads}G(Ox)}$$

CHE method uses reaction energies

$$\mathbf{O(ads) + H^+(aq) + e^-(U_{ads})}$$

$$\mathbf{\rightleftharpoons OH(ads),\ \Delta_{react} = 0 \Rightarrow U_{ads}}$$

Highlight

- similar predictions are obtained from these two approximate theories

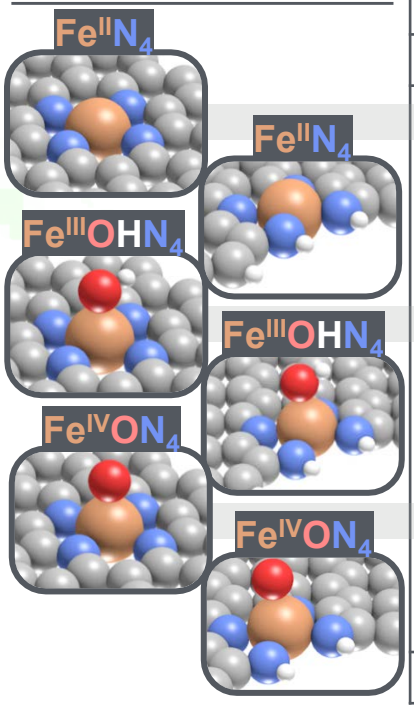
Accomplishments and Progress

Task 2.1: Active site modeling

The following mechanism is assumed with the given ΔG^0(eV) values to calculate the $\Delta_{ads}E$ in the LGER.

	Reaction	U^0(V)	ΔG^0(eV)
1.	$O_2(g) + H^+(aq) + e^- \rightarrow OOH(aq)$	-0.125	0.125
2.	$OOH(aq) + H^+(aq) + e^- \rightarrow O(aq) + H_2O(l)$	0.21	-0.21
3.	$O(aq) + H^+(aq) + e^- \rightarrow OH(aq)$	2.12	-2.12
4.	$OH(aq) + H^+(aq) + e^- \rightarrow H_2O(l)$	2.72	-2.72
5.	$O_2(g) + 4H^+(aq) + 4e^- \rightarrow 2H_2O(l)$	1.23	-4.92

Active sites considered



	O_2	OOH	O	OH	H_2O
Site	Adsorption Energy				
Fe^{II} bulk	-1.300	-2.160	-4.825	-3.074	-0.536
Fe^{II} edge	-1.053	-1.784	-4.273	-3.033	-0.490
Fe^{III} bulk	0.480	-2.429	-3.367	-2.095	-0.807
Fe^{III} edge	-0.207	-1.288	-2.864	-2.314	-0.365
Fe^{IV} bulk	-0.092	-1.058	-2.543	-1.616	-0.475
Fe^{IV} edge	-0.123	-0.805	-2.139	-1.625	-0.371
Ideal	0.0	-1.35	-2.49	-1.38	-0.0

Highlight

- $\Delta_{ads}E$ for III, IV states are closer to the ideal values

Note: $Fe^{III}OHN_4$ and $Fe^{IV}ON_4$ sites, adsorption is underneath the sheets

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Accomplishments and Progress

Task 2.1: Active site modeling

Reaction	Site											
	Fe^{II} bulk		Fe^{II} edge		Fe^{III} bulk		Fe^{III} edge		Fe^{IV} bulk		Fe^{IV} edge	
	Reversible Potential											
	LGER	CHE	LGER	CHE	LGER	CHE	LGER	CHE	LGER	CHE	LGER	CHE
1. $O_2(g) + H^+(aq) + e^- \rightarrow OOH(ads)$	2.87	2.89	1.66	1.68	2.30	2.33	1.16	1.19	**0.93**[a]	0.96	-	-
2. $OOH(ads) + H^+(aq) + e^- \rightarrow O(ads) + H_2O(l)$	2.04	1.29	1.15	1.95	1.15	**0.40**[a]	1.79	1.04	1.70	**0.94**[a]	1.54	-
Potential ranges where Fe^{IV} is stable												
3. $O(ads) + H^+(aq) + e^- \rightarrow OH(ads)$	0.37	0.70	0.88	1.21	0.85	0.69	1.57	1.90	1.19	1.52	1.61	1.94
Potential ranges where Fe^{III} is stable												
4. $OH(ads) + H^+(aq) + e^- \rightarrow H_2O(l)$	-0.35	0.04	-0.31	0.08	-	1.50	**0.41**[a]	**0.80**[a]	1.10	1.49	1.10	1.49

- The CHE method assigns the $H^+(aq)$ energy to ½ the calculated H_2 energy and adjusts the O_2 energy so that the calculated 4-electron reduction reaction energy is -4.92 eV. CHE predicts high activity for Fe^{III} edge and Fe^{IV} bulk sites

Highlight

- Both LGER and CHE theories predict activity for Fe^{III} and Fe^{IV} bulk sites
- Synthesis of engineered frameworks should shift focus to incorporation of Fe^{III} and Fe^{IV} sites.

[a] **Limiting potentials**

Accomplishments and Progress
Responses to Previous Year Reviewers' Comments

- This project was not reviewed last year

Collaborations

GreenWay Energy (Project Lead, Small Business)

- Prabhu Ganesan – material characterization, MEA fabrication, fuel cell testing, and project management
- Mark Elvington – rational design, synthesis, and development of engineered framework nano-scale electrocatalysts
- Alfred Anderson – direct the active site modeling

SRNL (Subcontractor, FFRDC)

- Héctor Colón-Mercado – electrochemical characterization, catalyst activation, and fuel cell testing

Northwestern University (Subcontractor, University)

- Joseph Hupp – manage NU polymer electrocatalyst design and synthesis
- Omar Farha – direct NU polymer electrocatalyst design and synthesis

Ballard Power Systems (OEM, Industry)

- Shanna Knights – evaluation of promising electrocatalysts

ElectroCat Consortium Collaborations

Los Alamos National Laboratory (Capable Laboratory)

- Piotr Zelenay, Hoon Taek Chung
  - Membrane electrode assembly fabrication
  - PGM-free catalyst synthesis, analytical characterization, electrochemical and fuel cell testing
- Edward Holby
  - Multi-scale modeling for rational design of PGM-free catalysts

Oak Ridge National Laboratory (Capable Laboratory)

- Karren More
  - Analytical electron microscopy and/or electron tomography
    (Collaboration begins during year 2)

Remaining Challenges and Barriers

Task 1 – Catalyst development based on high surface area polymers

- All Subtasks – Catalysts require heat treatment for optimal ORR performance
- All Subtasks – Catalysts require improvement to long term stability
- Subtask 1.1 – CTF metal loading and heat treatment requires optimization
- Subtask 1.2 – Surface area of polyporphyrins slightly low (~900 m^2/g)
- Subtask 1.3 – N-doped carbon requires increased activity

Task 2 – Active site modeling

- Subtask 2.2 – The kinetic treatment on the combined electron transfer and bond rearrangement presents a challenge. This form of OOH(ads) may be important to understanding active site degradation and poisoning.

Task 3 – MEA optimization and fuel cell testing

- Subtask 3.1 – Optimize MEA fabrication to decrease HFR and increase catalyst utilization

Proposed Future Work

Task 1 – Catalyst development based on high surface area polymers

- Catalysts based on "phen" type functionalities
  - Materials will continue to be optimized and tested in the next quarter
- Catalysts based on porphyrinic type functionalities
  - Continue optimizing the catalyst by adding peripheral groups and different heteroatoms
  - Explore use of different transition metal centers
- Catalysts based on high N content
  - Continue optimization studies
- Down select promising catalysts for MEA optimization

Task 2 – Active site modeling

- Align and validate models against experimental materials

Task 3 – MEA optimization and fuel cell testing

- Initiate in-house FC screening of prepared catalyst
- Continue FC optimization at LANL

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

Summary

- A bottom-up approach was used to prepare PGM-free Engineered Framework Nano-Structure Catalysts with "phen" type active sites (e.g. CTFs, YSNs, and MOFs) and porphyrinic type active sites (MOFs and POPs).
- Electrochemical characterization shows high performance for the ORR (see table)
- A highly scalable process has been developed to produce inexpensive, high N, carbon based PGM-free catalysts designed to maximize N content, control pyridinic/pyrrolic N content, and maximize surface area
- Modeling studies strongly suggest bulk Fe^{IV} has promise for catalyzing the four-electron reduction of O_2 to water since its predicted overpotential of 0.29 V is the lowest.
  - Edge Fe^{III} has similar reactivity with a 0.43 V predicted overpotential. No other sites are active.
  - The dissociated structure of OOH(ads) with OH binding to C and O to Fe seen for bulk Fe^{III} and Fe^{IV} sites has not been discussed previously for carbon-based catalysts.

Metric	Units	Current Status	FY18 Target	FY19 Target	FY20 Target	2020 DOE Target
Fuel Cell test: Catalyst Activity	mA cm^{-2} @ 900 $mV_{IR\text{-}free}$	---	≥ 20[b]	≥ 25[b]	≥ 30[b]	≥ 44[a]
Fuel Cell test: Catalyst Activity	mA cm^{-2} @ 800 mV	**52.8**	NA	NA	≥ 150[c]	NA
RRDE test: Catalyst Activity	mA cm^{-2} @ 800 mV	**2.03**	≥ 1.5[d]	≥ 2.0[d]	NA	NA

[a] 80°C H_2/O_2 MEA; fully humidified, total outlet pressure 150 kPa; anode stoich 2; cathode stoich 9.5
[b] 80°C H_2/O_2 in an MEA; total outlet pressure of 100 kPa
[c] 80°C H_2/Air in an MEA; total outlet pressure of 100 kPa
[d] 0.1 M $HClO_4$ acid; catalyst loading of 0.6 mg cm^{-2}

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Acknowledgements

Project Management and Review

Donna Ho, DOE

Adria Wilson, DOE

Dimitrios Papageorgopoulos, DOE

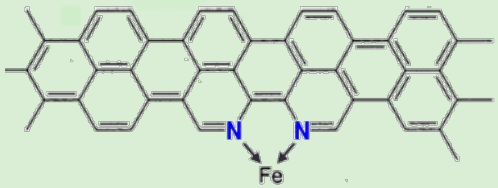
John Kopasz, ANL

ElectroCat Steering Commitee and Experts

ElectroCat Project PIs

Technical Backup Slides

Key theories for designing non-PGM catalysts



❖ Proposed catalyst composition FeN_2C_y carbon catalyst

- Comparison of catalytic activity (V_{pr}) and relative abundance of FeN_xC_y species

Analysis of FeN_xC_y functional groups through RDE and ToF SIMS identifies FeN_2C_y and FeN_4C_y sites as catalytically active for the ORR

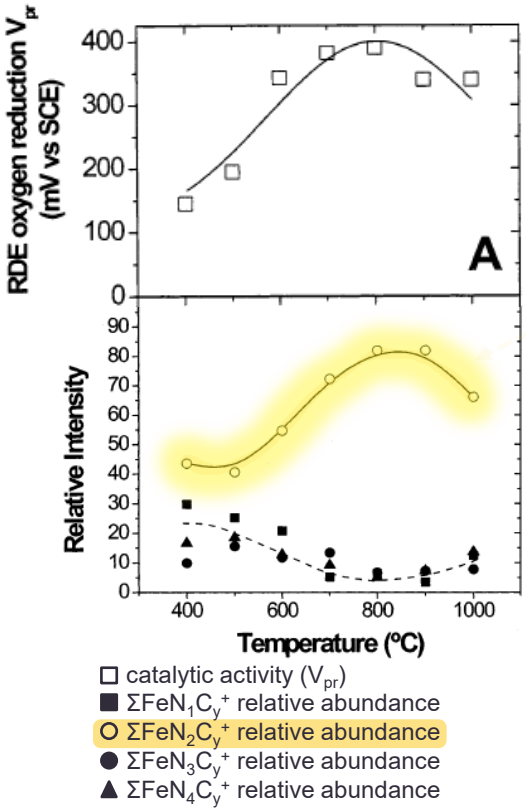
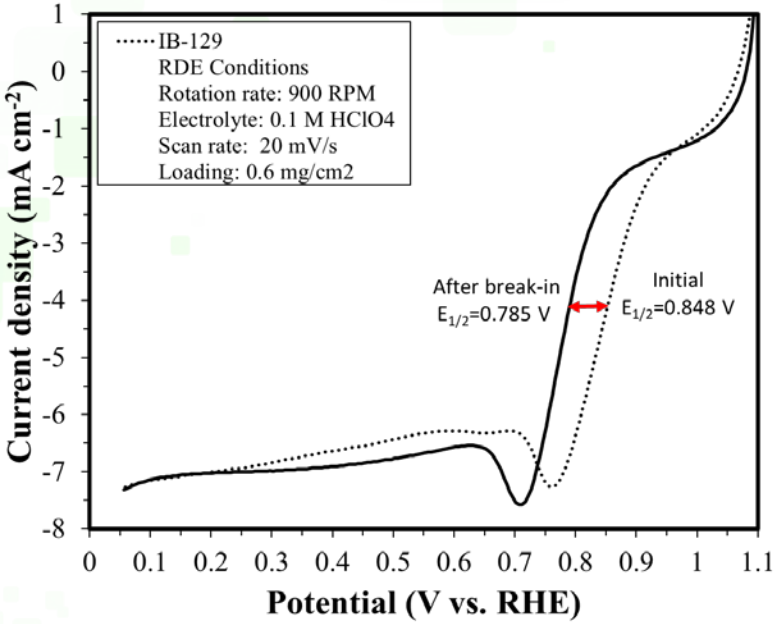


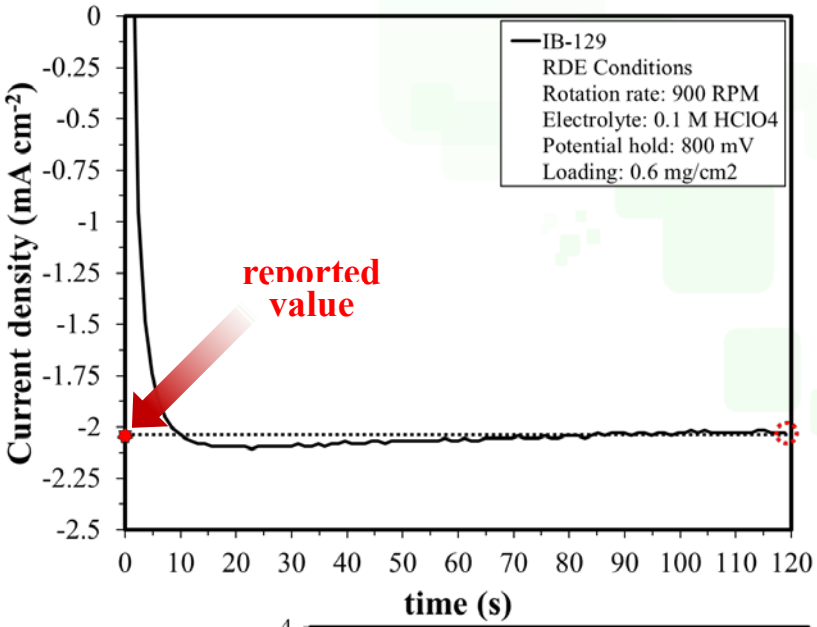
TABLE 1: Relative Abundance in % of $FeN_xC_y^+$ Ions as a Function of the Pyrolysis Temperature for Type II Fe(0.2)Ac Catalysts

ions	400 °C	500 °C	600 °C	700 °C	800 °C	900 °C	1000 °C
$FeNC^+$	28.27	23.82	17.08	0.76	5.76	1.77	2.50
$FeNC_2^+$	0.78	0.00	1.61	2.63	0.00	0.40	2.50
$FeNC_3^+$	0.78	1.41	2.06	1.82	0.63	1.33	7.50
FeN_2C^+	14.94	7.78	4.80	2.38	1.56	2.56	3.75
$FeN_2C_2^+$	1.78	4.70	1.44	0.53	0.63	0.83	0.00
$FeN_2C_3^+$	0.40	1.26	0.53	1.85	0.00	0.93	12.50
$FeN_2C_4^+$	23.92	26.93	46.95	64.89	78.38	76.38	49.86
$FeN_2C_5^+$	1.10	0.00	0.35	2.08	0.00	0.93	0.00
$FeN_2C_6^+$	1.47	0.00	0.64	0.53	1.32	0.40	0.00
FeN_3C^+	1.75	4.97	5.68	1.32	0.00	0.00	2.78
$FeN_3C_2^+$	0.00	1.36	0.00	0.00	1.32	0.42	0.00
$FeN_3C_3^+$	1.78	2.98	1.91	1.82	0.00	0.81	2.78
$FeN_3C_4^+$	0.00	1.10	0.00	1.06	0.00	0.00	0.00
$FeN_3C_5^+$	2.33	0.37	0.29	0.53	1.56	0.85	0.00
$FeN_3C_6^+$	2.64	0.47	0.35	0.76	1.56	0.00	2.78
$FeN_3C_7^+$	0.00	0.00	0.00	0.00	0.00	0.42	0.00
$FeN_3C_8^+$	0.81	3.98	3.36	2.89	0.00	1.67	1.25
$FeN_3C_9^+$	7.33	3.29	1.16	0.76	0.63	3.06	4.03
FeN_4C^+	3.01	0.68	1.12	1.32	0.00	0.42	0.00
$FeN_4C_2^+$	0.34	1.31	1.67	2.38	0.00	0.93	0.00
$FeN_4C_3^+$	0.34	1.89	0.00	0.76	1.56	0.42	0.00
$FeN_4C_4^+$	0.72	0.52	1.08	0.00	0.00	0.42	2.50
$FeN_4C_5^+$	0.40	0.37	2.18	1.32	1.56	0.00	0.00
$FeN_4C_6^+$	0.00	0.00	0.00	0.53	0.00	0.40	1.25
$FeN_4C_7^+$	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$FeN_4C_8^+$	5.08	8.05	5.45	4.17	1.88	4.64	4.03
$FeN_4C_9^+$	0.00	1.72	0.29	1.60	0.00	0.00	0.00
$FeN_4C_{10}^+$	0.00	0.68	0.00	0.00	0.00	0.00	0.00
$FeN_4C_{11}^+$	0.00	0.00	0.00	1.32	0.00	0.00	0.00
$FeN_4C_{12}^+$	0.00	0.37	0.00	0.00	1.67	0.00	0.00

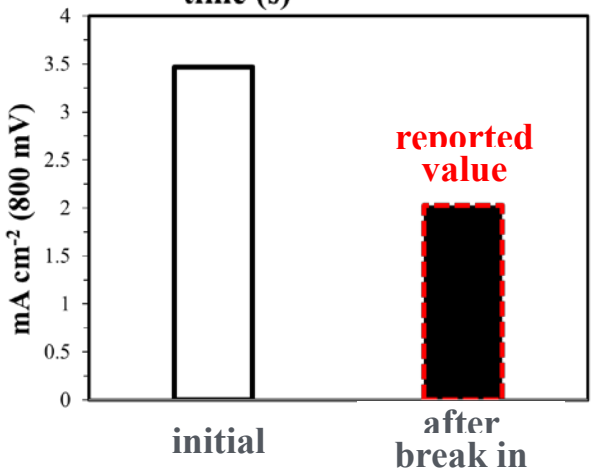
J. Phys. Chem. B **2002,** *106,* 8705-8713

Project's Electrochemical Screening Protocol



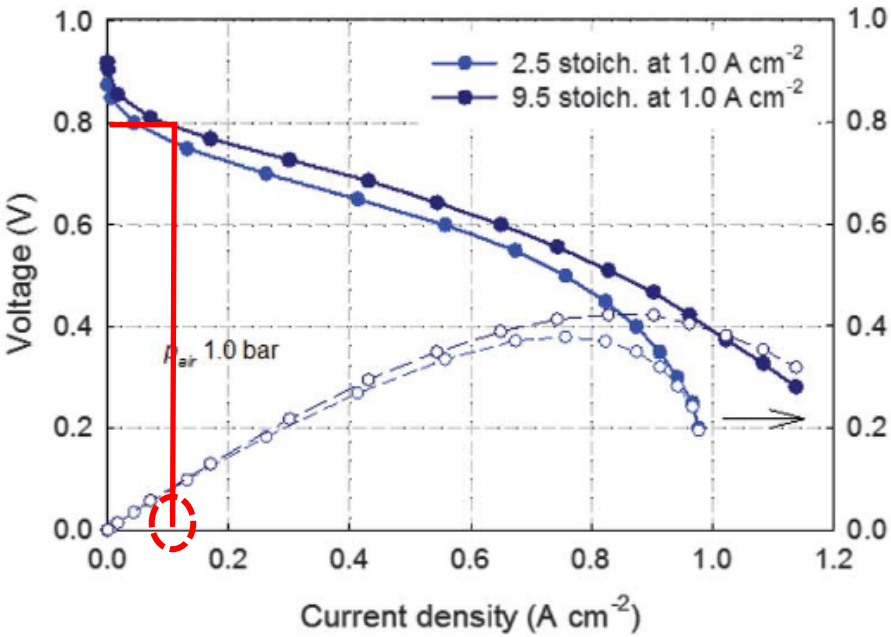
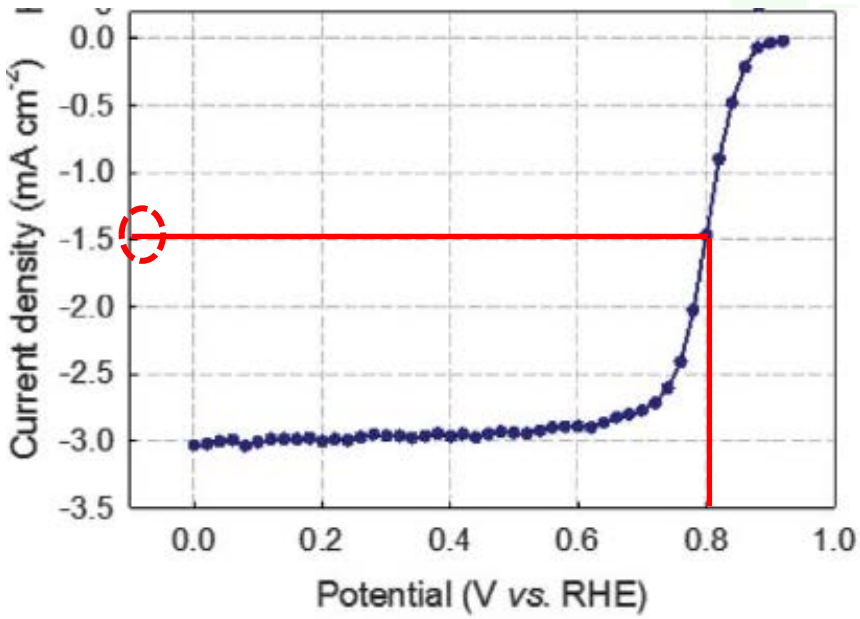


- RRDE Electrochemical Screening Procedure
  1.) Cyclic Voltammetry – 50 full cycles under O_2 (break in)
  2.) Cyclic Voltammetry – 2 full cycles at 900 rpm and 2 full cycles at 1600 rpm
  3.) Chronoamperometry – 2 minutes at 800 mV vs RHE. Current measured at 2 minutes is the reported value.



FC and RRDE State of the art performance

Work published in Science by Zelenay and team [Chung et al., Science 357, 479–484 (2017)].

- FC current at 800 mV is **~100 mA/cm²**
- RDE current at 800 mV is **~1.5 mA/cm²**

Project targets (assigned by FCTO in FC, as well as our internal targets for RDE) agree well with demonstrated values of the state-of-the-art catalysts.