Developing Platinum Group Metal-Free Catalysts for Oxygen Reduction Reaction in Acid: Beyond the Single Metal Site

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Project ID# FC302

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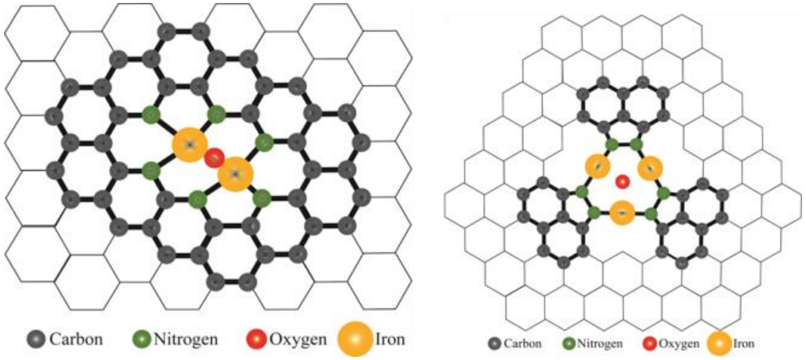


Northeastern University
Center for Renewable Energy Technology

BERKELEY LAB

Overview

Timeline

- Project Start Date: 10/01/2018
- Project End Date: 03/31/2021

Barriers

- Performance in PEMFCs
- Durability in PEMFCs

Budget

- Total Project Budget: $1,020,000.00
  - Total Recipient Share: $250,000.00
  - Total Federal Share: $770,000.00
  - Total DOE Funds Spent*: $460,397.86

* As of 05/25/2020

Partners

- Lawrence Berkeley National Laboratory
  Adam Weber
- Northeastern University
  Sanjeev Mukerjee
- Project lead
  Qingying Jia (NEU)

Relevance

Objectives: Development of PGM-free ORR catalysts with high performance and durability in PEMFCs.

- Development of M_x-N-C catalysts featured with multiple metal centers (MMCs).
- Synthesis of $M_{(x)}$-N-C catalysts via surface deposition methods to bypass the necessity of pyrolysis.

Relevance: Our approaches move beyond the M-N-C catalysts featured with single metal sites and traditional synthesis routes pyrolyzing the mixture of metal, N, and C precursors. The new catalysts may address the limited activity, durability, and active site density of M-N-C catalysts and meet the DOE targets.

Targets:

- 0.035 A/cm^2 at 0.9 V in a H_2-O_2 PEMFC (1.0 bar partial pressure, 80°C)
- Loss in activity ≤ 40% after 30,000 square wave cycles with steps between 0.6 V (3 s) and 0.95 V (3 s) .
- Power density of 0.5 W/cm^2 in a H_2-Air PEMFC with a MEA size ≥ 50 cm^2

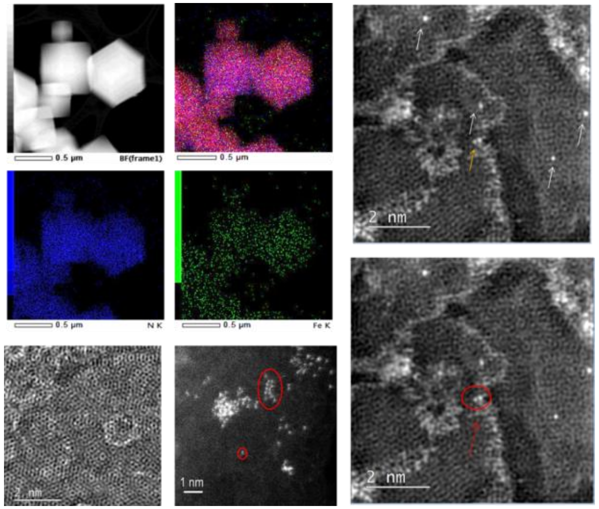
Approach and Targets

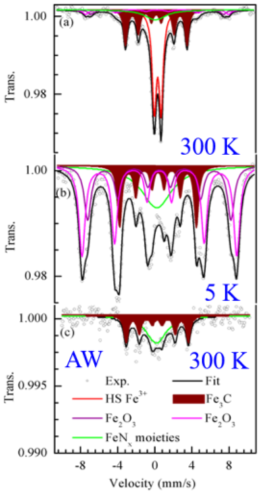
- Synthesis
  1. Ionothermal Carbonization (abandoned)
  2. Chemical vapor deposition (CVD)
  3. Ion Beam-Assisted Deposition (IBAD)
  4. Flash pyrolysis
- Characterizations
  Spectroscopy: *in situ* XAS, Mossbauer, XPS, NMR, XRD
  Microscopy: SEM, HAADF-STEM, HRTEM
- MEA fabrication
  electrospinning, IBAD
- Mass transport modeling
- Milestones
  1. 0.025 A/cm^2 at 0.90 V in a H_2/O_2 PEMFC (Period 1 Go/No-Go)
  2. Loss in activity ≤ 40% after 30,000 square wave cycles
  3. Power density of 0.5 W/cm^2 in a H_2/Air PEMFC

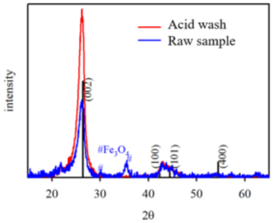
Accomplishments and Progress

Ionothermal Carbonization synthesis (ceased)

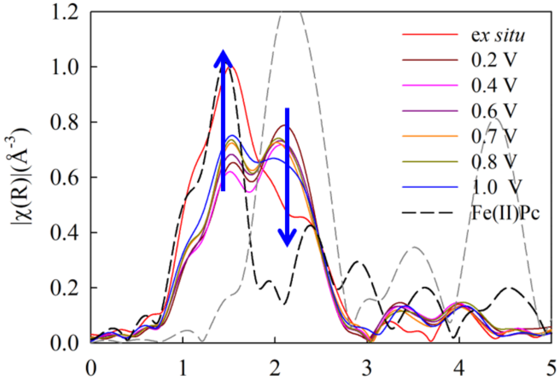
NaCl+$ZnCl_2$ (1:7 by wt) as molten salt; adenine as C and N precursor; $Fe(Phen)_3(ClO_4)_2$ as Fe precursor (Fe-N_6)

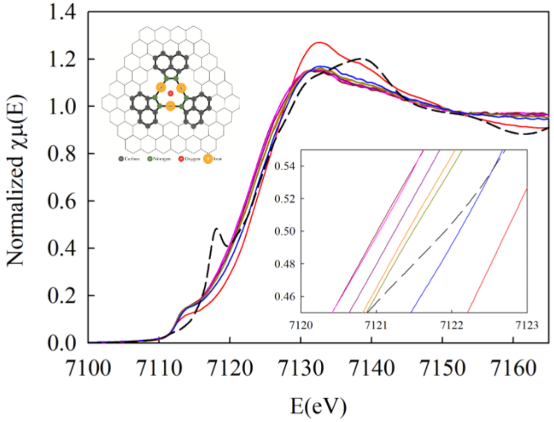


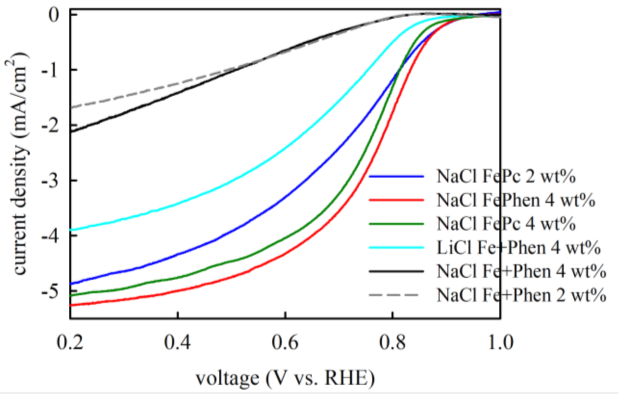




Sample	Mössbauercomponent	Mössbauer RA % (300 K)	Mössbauer RA % (5 K)
ICM-$FePhen_3$	Singlet	12	22
	Fe_2O_3 (1)	58	62
	Fe_3C	30	16
ICM-$FePhen_3$-AW	Singlet	55	NA
	Fe_2O_3 (1)	0	NA
	Fe_3C	45	NA

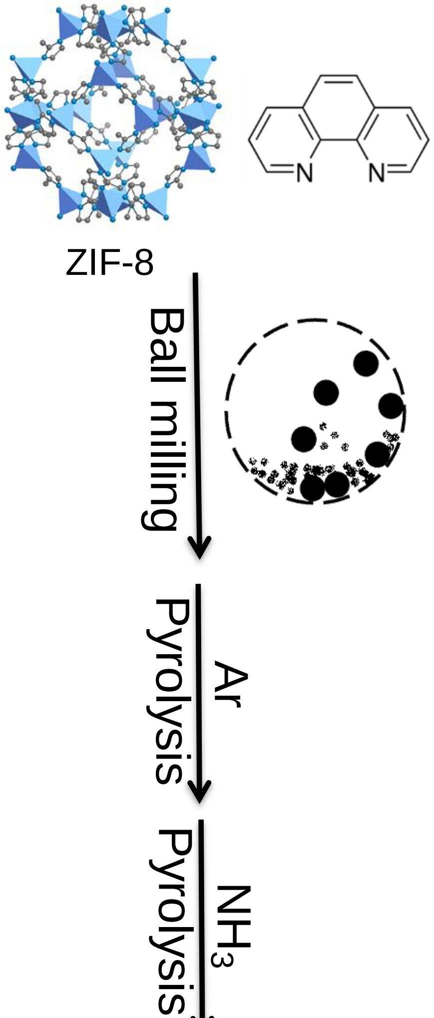




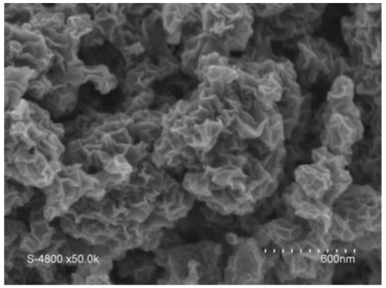


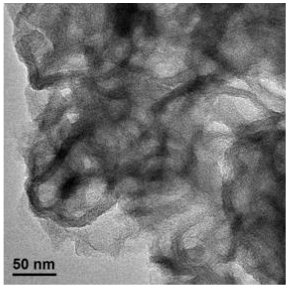
Combined characterizations show the presence of electrochemically active MMC sites in the M_x-N-C catalysts, but poor ORR activities in RDEs.

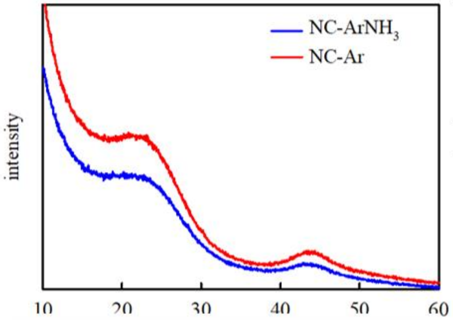
Synthesis of microporous N-C substrate without iron

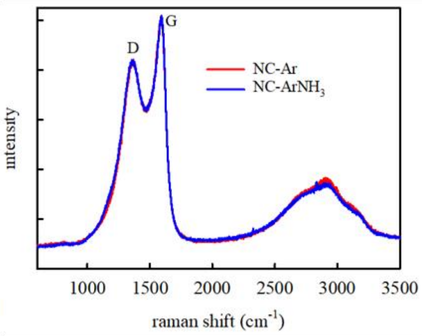


N-C

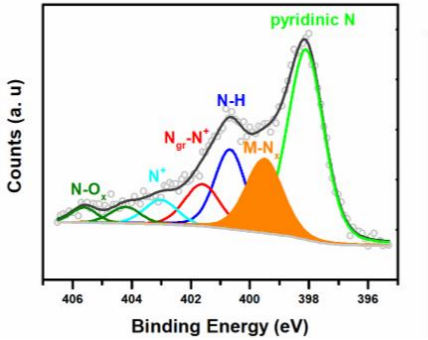


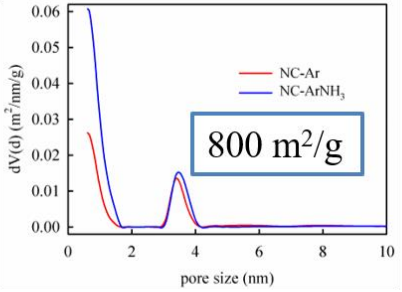






Highly porous N-doped carbon substrate with abundant micropores and enriched pyrindic N content was produced for in-temperature XAS studies and for deposition methods.





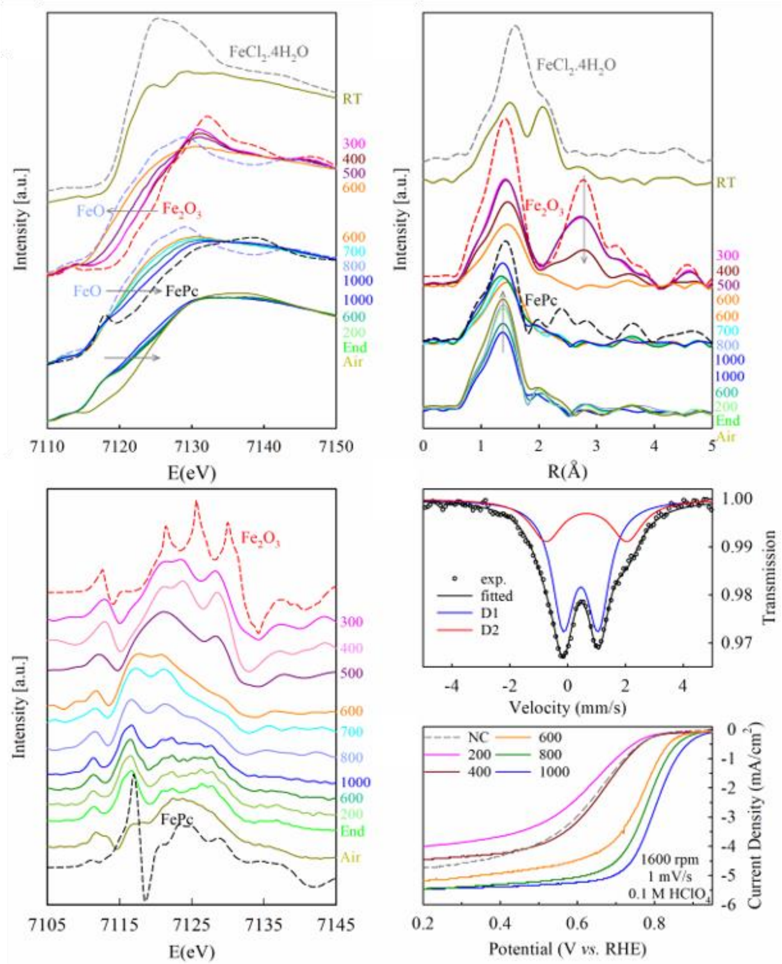
Jia *et al.*, JACS, **2019**

Highly microporous and well-defined N-C substrate was achieved.

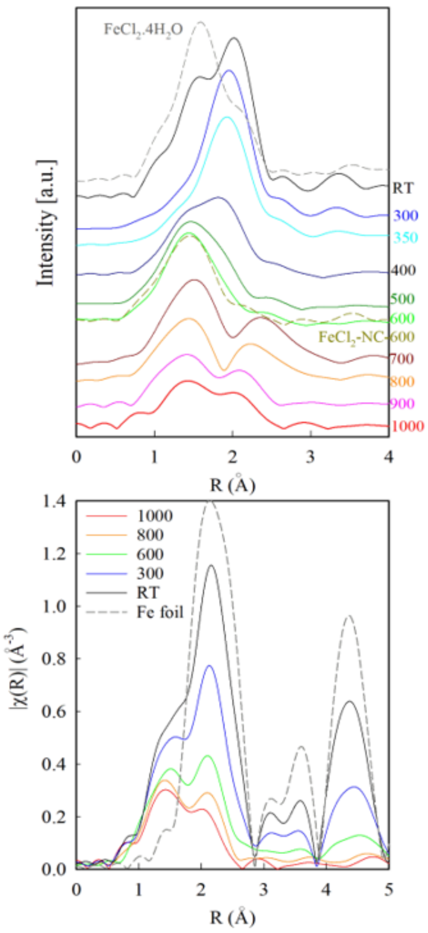
Accomplishments and Progress

In-temperature XAS characterizations

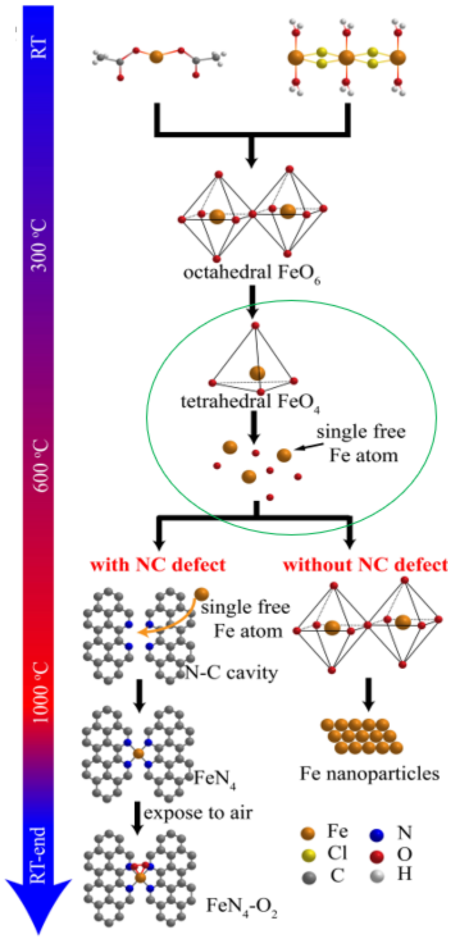
FeCl$_2$·4H$_2$O + N-C



FeCl$_2$·4H$_2$O + SiO$_2$



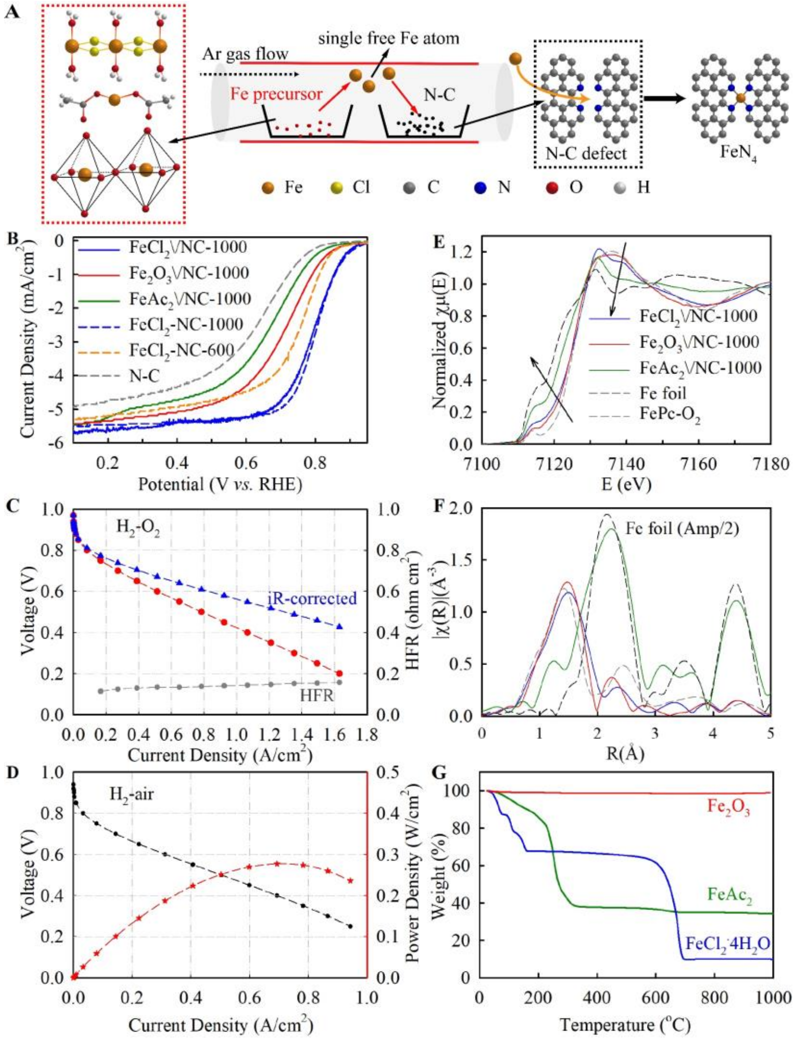
Jia *et al.*, JACS, **2019**

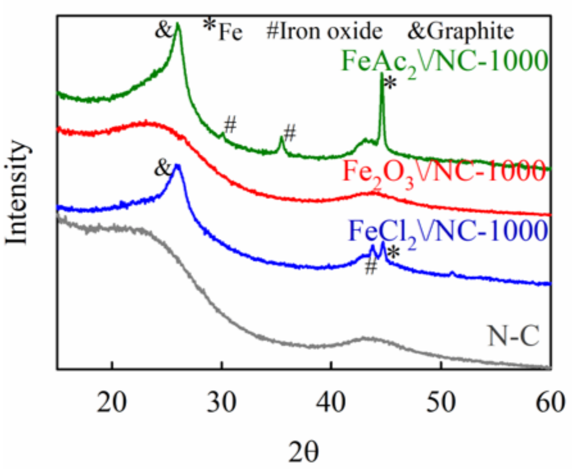


In-temperature XAS reveals the stepwise formation of Fe-N$_4$ sites during pyrolysis.

Accomplishments and Progress

Non-contact pyrolysis





Residual powders in the Fe boat.

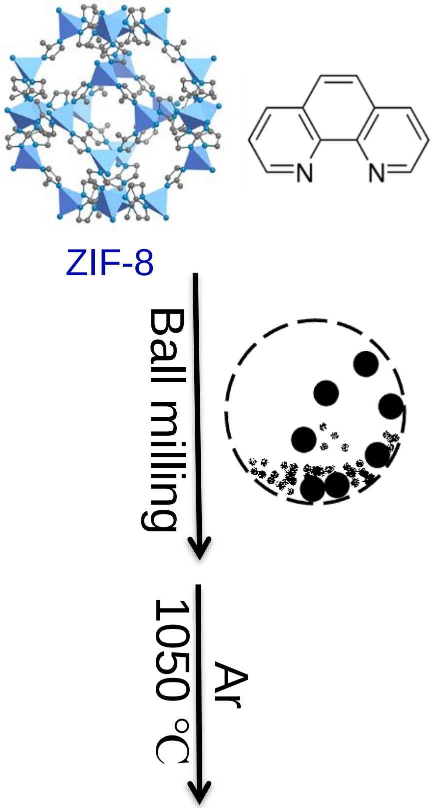
Inspired by the evolution pathway of Fe-N_4 sites (Fe-O_4 → Fe_1 (g) → Fe-N_4) that involves diffusion of gaseous Fe_1, we initiated non-contact pyrolysis.

Three representative Fe precursors with distinctly different evaporation temperatures and N-C substrate were placed in two separate bolts during pyrolysis:

$FeCl_2 \cdot 4H_2O$: abundant Fe-N_4 sites formed
$FeAc_2$: no Fe-N_4 sites but Fe nanoparticles formed
Fe_2O_3: trace amounts of Fe-N_4 sites formed

Synthesis of Fe-N-C catalysts with Fe-N_4 sites via non-contact pyrolysis is demonstrated.

N-C substrate for chemical vapor deposition (CVD)



ZIF-8

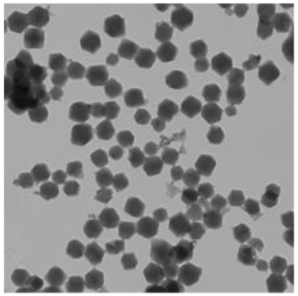
Ball milling

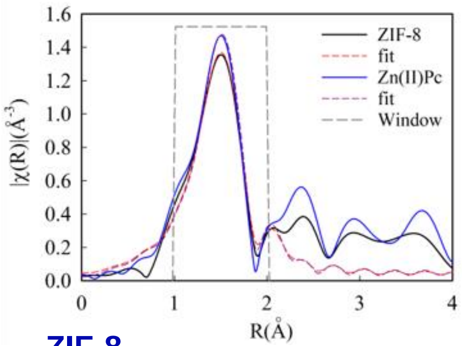
1050 °C

Ar

N-C

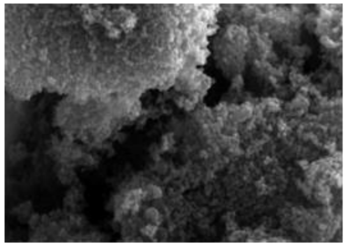
No NH_3 pyrolysis

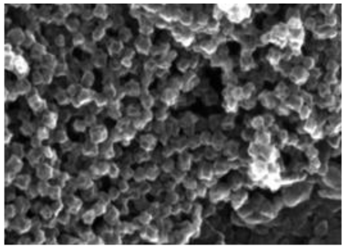




ZIF-8

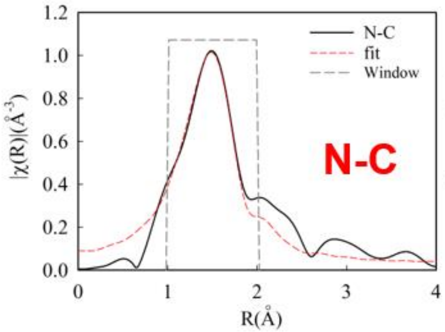
In-house ZIF-8 has an average particle size of ~80 nm, dominated by Zn-N_4.

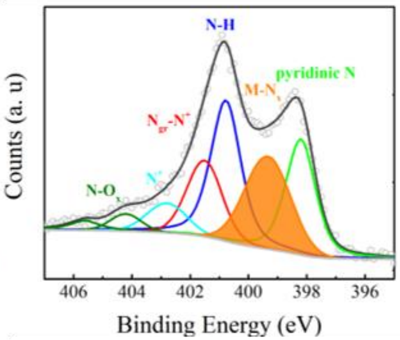




FT-EXAFS fit

Zn-N bond	R (Å)	N
ZIF-8	1.99(1)	4.1(5)
Zn(II)Pc	1.98(1)	3.8(8)
N-C	2.00(1)	4.8(5)





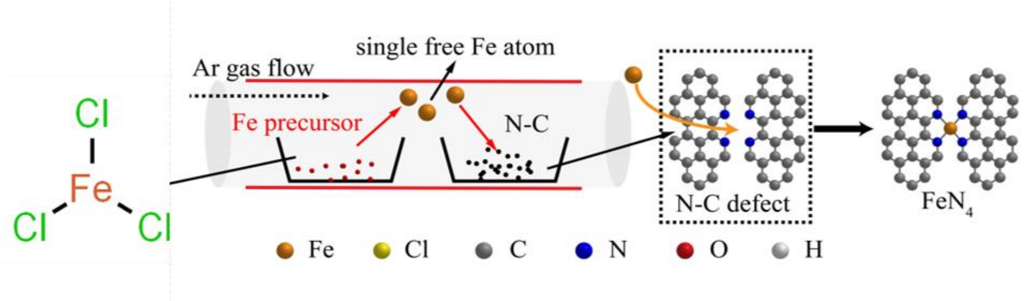
Zn-N_4 structure and particle size are retained upon pyrolysis.

N-C is composed of Zn-N_4 sites embedded in highly porous carbon matrix.

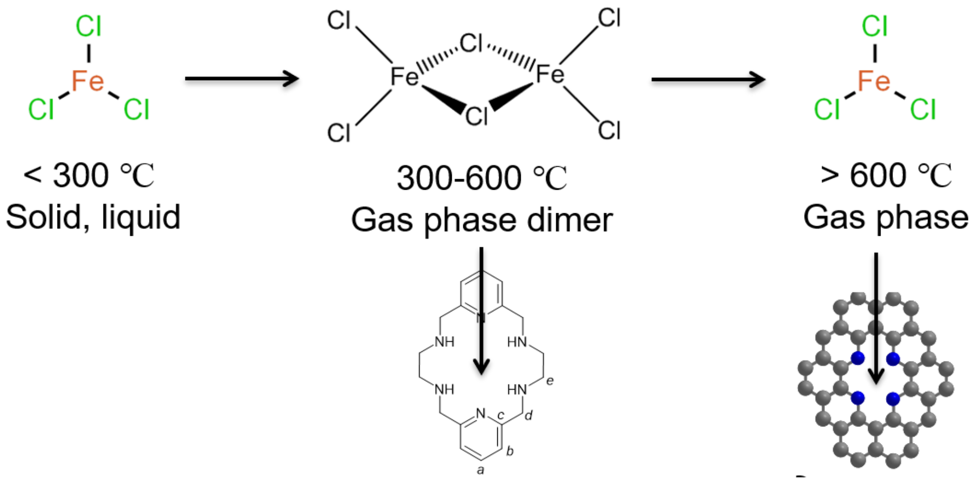
Make new N-C substrate from in-house ZIF-8 with optimized particle size.

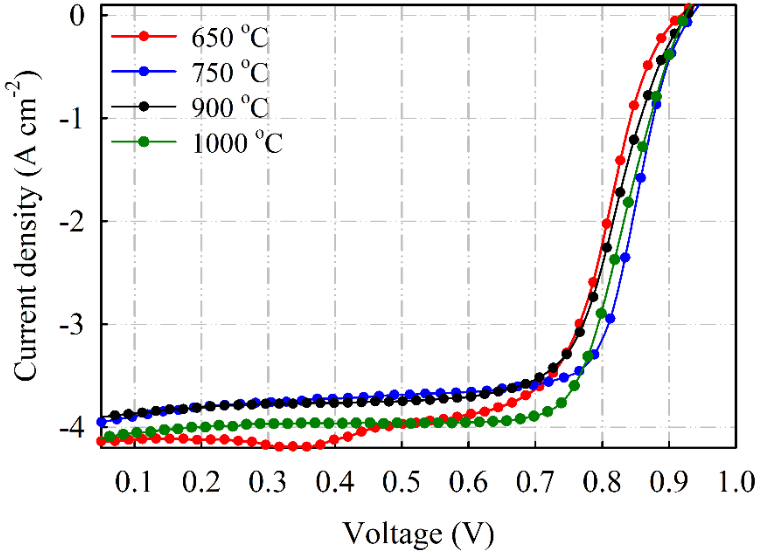
Accomplishments and Progress

Chemical vapor deposition (CVD)



ICP	Fe	Zn	N	C
N-C	-	2.16	4.23	84.00
FeNC-CVD-650	2.25	1.05	3.97	85.42
FeNC-CVD-750	**2.00**	0.12	4.24	85.48
FeNC-CVD-900	3.76	0.23	3.32	85.42
FeNC-CVD-1000	2.72	0.03	2.36	84.20





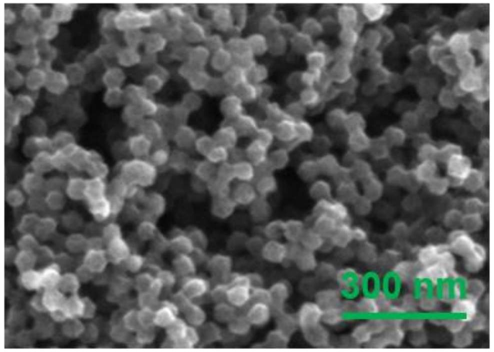
CVD method is demonstrated by using anhydrous $FeCl_3$, taking advantage of its low evaporation temperature. It holds the potential to make Fe_2-N_x-C sites signified by the gaseous Fe_2Cl_6 at 300-600 ℃.

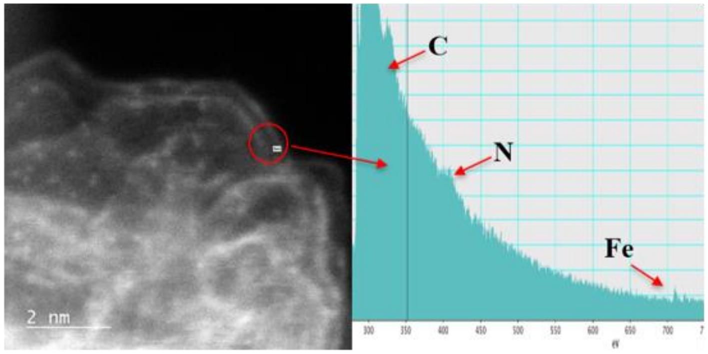
Among a wide temperature range 750 ℃ gives the best ORR activity in a RDE.

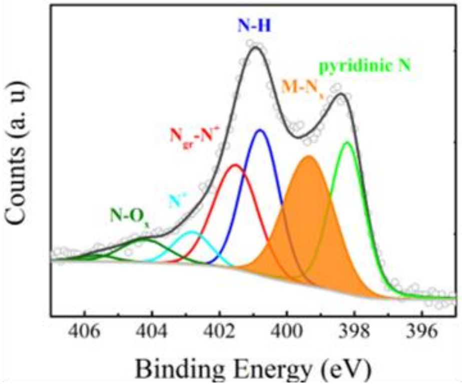
CVD method produces highly active Fe-N-C catalysts for the ORR.

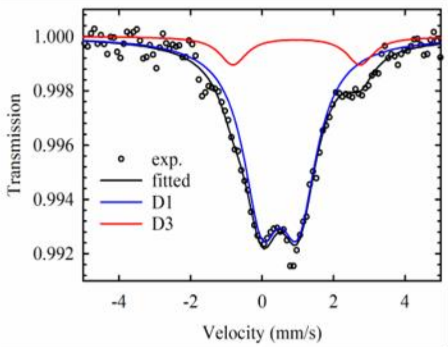
Accomplishments and Progress

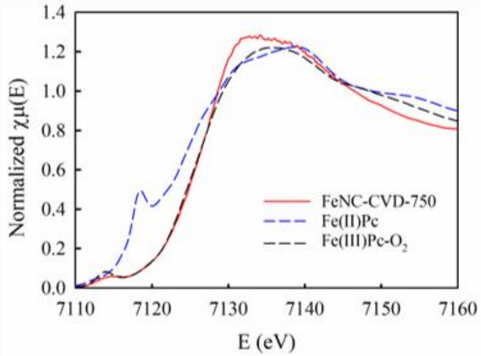
CVD: *ex situ* characterizations

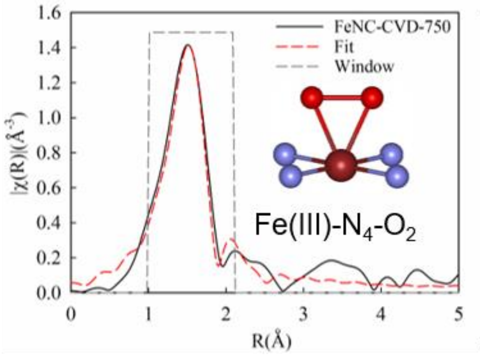


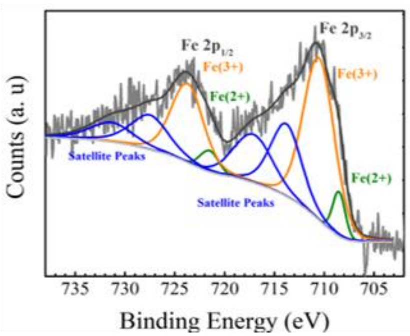












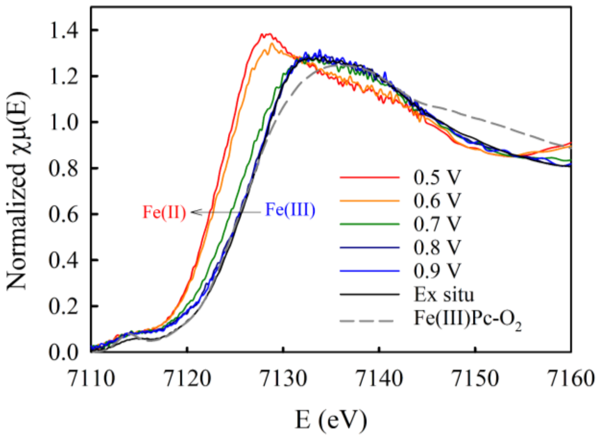
Comp.	RA %	IS mm s^{-1}	QS mm s^{-1}	LW mm s^{-1}	Assignment
Doublet 1	89	0.50	1.02	1.25	Fe(III)-N$_4$-O$_2$
Doublet 3	11	0.97	3.56	0.92	$FeCl_2$

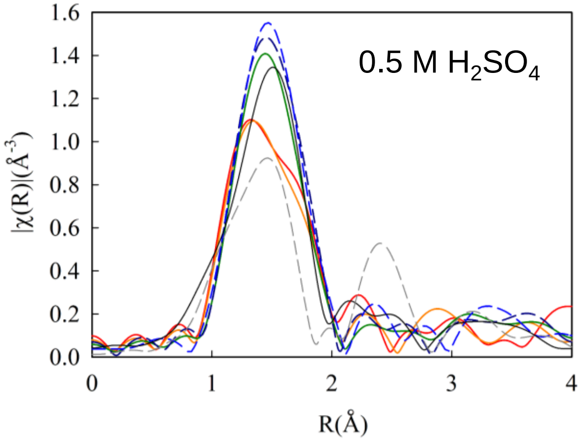
Multiple *ex situ* characterizations converge to the conclusion that the FeNC-CVD-750 contains predominately (~90%) Fe(III)-N$_4$-O$_2$ (D1) species and is absent of Fe(II)-N$_4$ (D2).

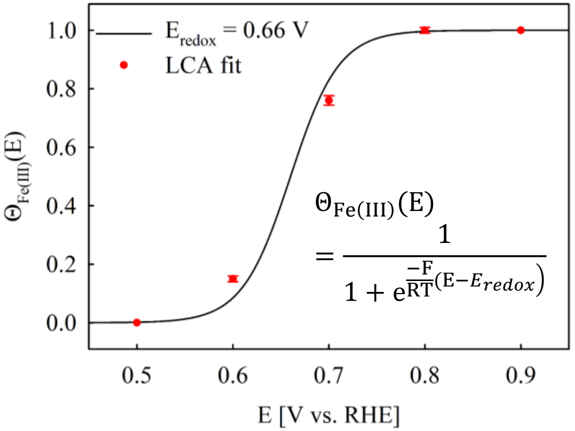
All Fe(II)-N$_4$ sites in FeNC-CVD-750 located on surface in the form of Fe(III)-N$_4$–O$_2$.

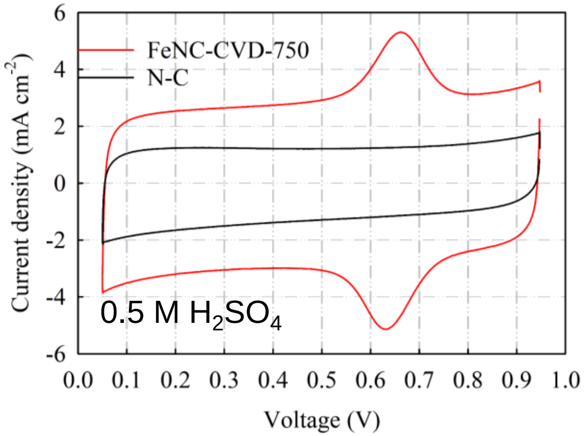
Accomplishments and Progress

CVD: *in situ* XAS characterizations









$$Fe(III)\text{-}N_4\text{-}O_2 \leftrightarrow Fe(II)\text{-}N_4$$

In situ XAS identifies the Fe(III)/Fe(II) redox transition at 0.66 V vs RHE, consistent with the *CV*. It further identifies all Fe(II)-N_4 sites are electrochemically active towards the ORR.

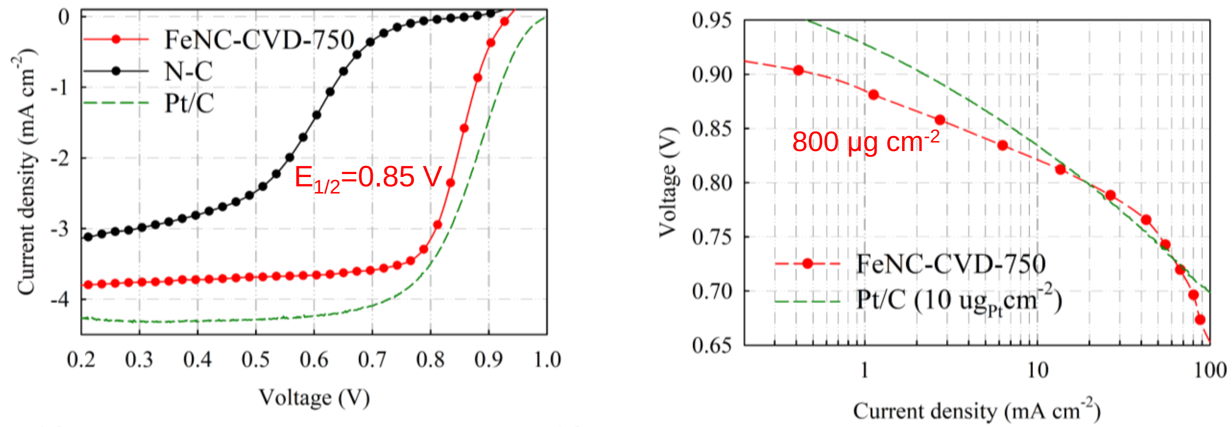
FeNC-CVD-750 contains predominately Fe-N_4 sites with ~1.8 wt_{Fe}% that are all located on surface accessible by air, corresponding to nearly 100% Fe-N_4 utilization or ~90% Fe utilization (~10% residual $FeCl_2$). This is distinctly different from previous Fe-N-C catalysts that contain both exposed (D1) and buried Fe-N_4 (D2) sites.

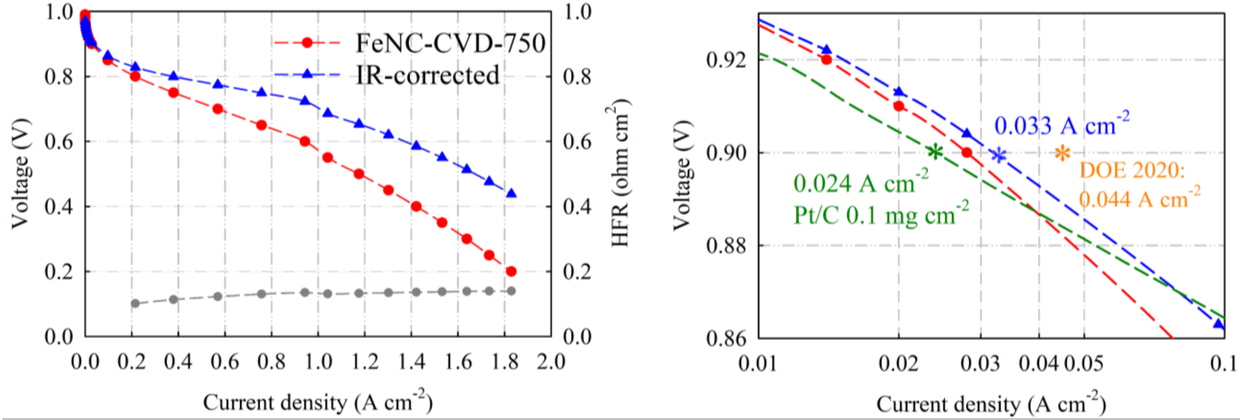
By CVD method, Fe-N_4 sites are formed at locations accessible by gaseous $FeCl_3$. They are thus accessible by air. Whereas in previous methods the sufficient mixing of Fe, N, C precursors prior to pyrolysis makes the Fe-N_4 formed and distributed throughout the carbon matrix.

Nearly 100% utilization of Fe-N_4 sites (1.8 wt_{Fe}%) is identified *in situ*.

Accomplishments and Progress

CVD: ORR activity assessments





In a RDE, the FeNC-CVD-750 (800 μg cm^{-2}) exhibits a half-wave potential of 0.85 V in 0.5 M H_2SO_4, and a kinetic current density comparable to that of Pt/C (TKK, 10 μg cm^{-2}) in 0.1 M $HClO_4$.

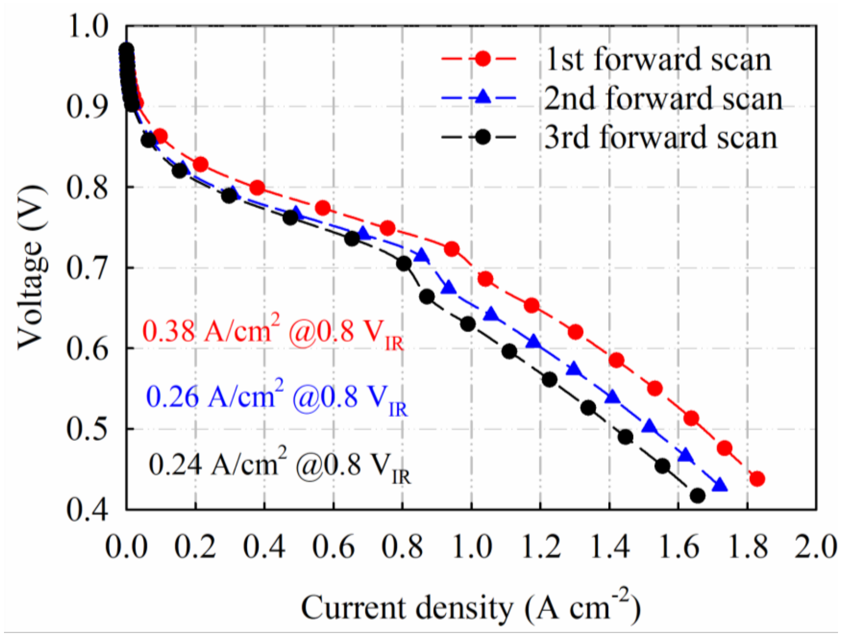
In a H_2-O_2 PEMFC, the FeNC-CVD-750 (6 mg·cm^{-2}) delivers a current density of 0.033 A·cm^{-2} at 0.9 V, surpassing Budget Period 1 Go/No-Go Decision Point of 0.025 A·cm^{-2}, and that (0.024 A·cm^{-2}) of Pt/C (TKK, 0.1 mg·cm^{-2}).

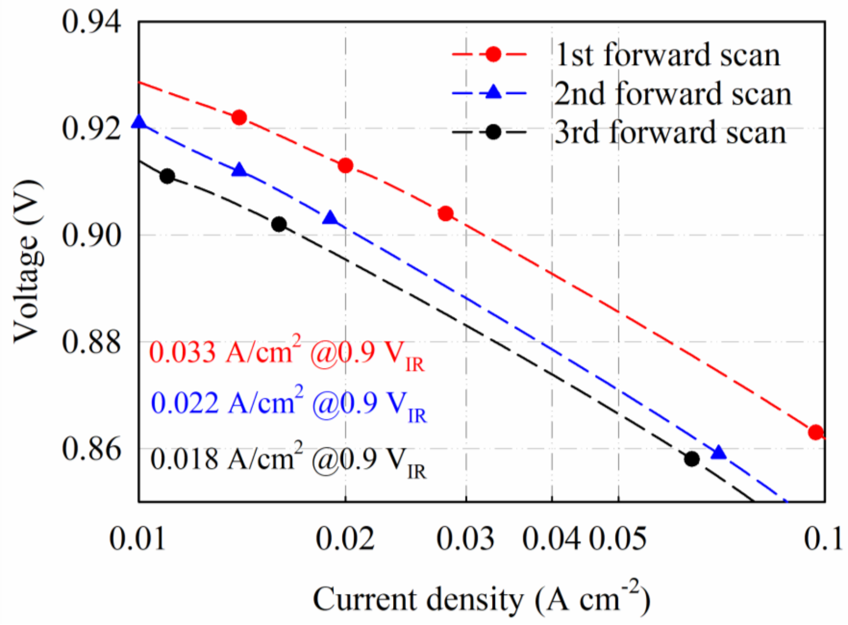
5 cm^2 MEA; Cathode: 6 mg/cm^2, Anode: 0.3 mg$_{Pt}$/cm^2; H_2: 200 ml/min; O_2: 200 ml/min; P_{O2} = P_{H2} = 1 bar partial pressure, 100% relative humidity (RH), 80 ℃; Nafion-212. Conducted by Giner Inc.

FeNC-CVD-750 delivers 0.033 A·cm^{-2} at 0.9 V in H_2-O_2 PEMFCs.

Accomplishments and Progress

CVD: PEMFC durability



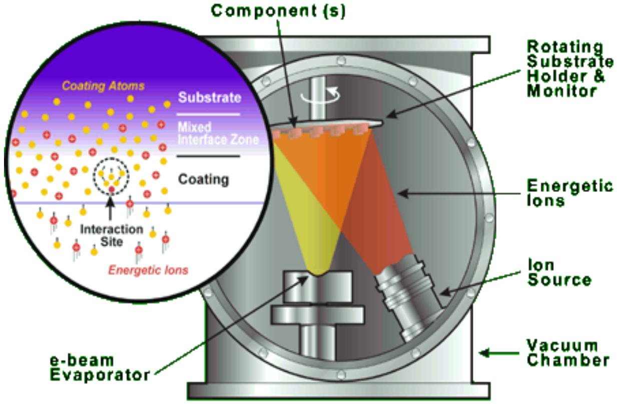


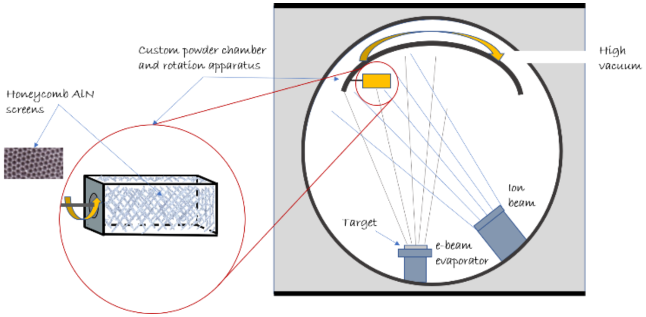
The current density @ 0.8 V degrades **~ 37%** at the third scan.
The current density @ 0.9 V degrades **~ 45%** at the third scan.
Major loss occurs upon the first scan.

FeNC-CVD-750 is not durable in H_2-O_2 PEMFCs.

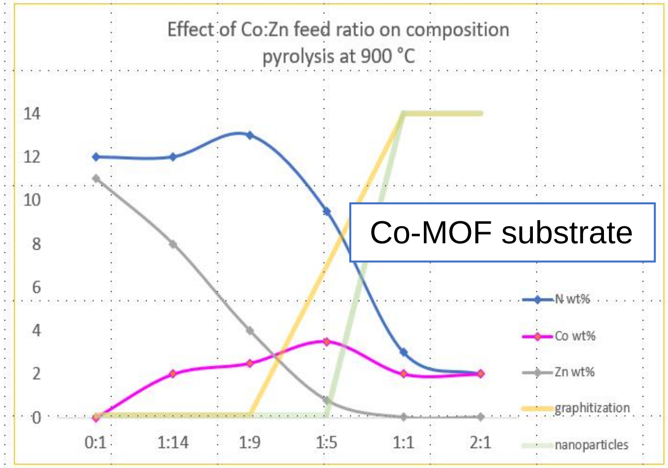
Accomplishments and Progress

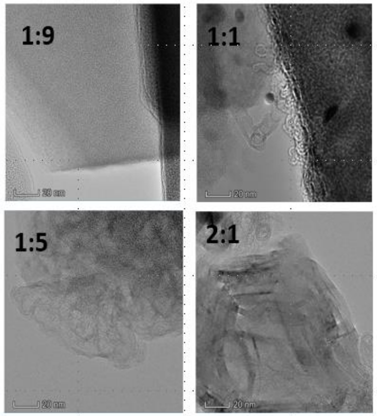
IBAD: RT-deposition of Fe metal onto Co-MOF substrate

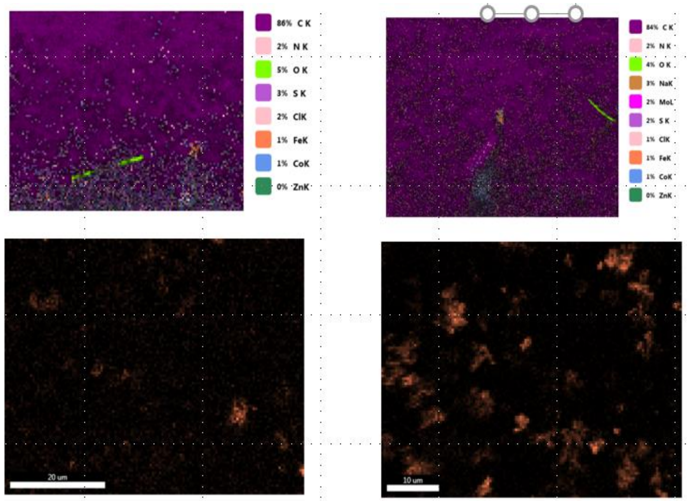




IBAD adjusted to enable metal deposition on powder substrate







Metallic Fe is deposited on Co-MOF. Next step is to deposit single-atom Fe.

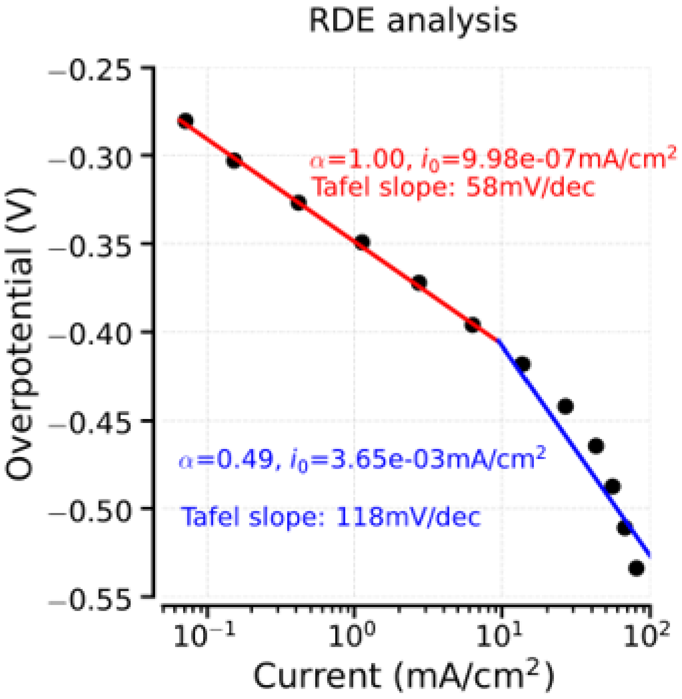
Deposition of Fe metal onto Co-MOF substrate by IBAD at RT is achieved.

Accomplishments and Progress

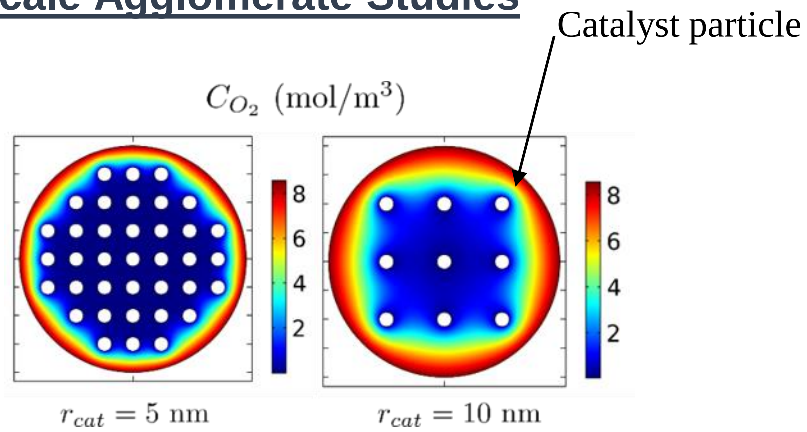
Non-PGM MEA Kinetics & Microscale modeling

Kinetics modeling:

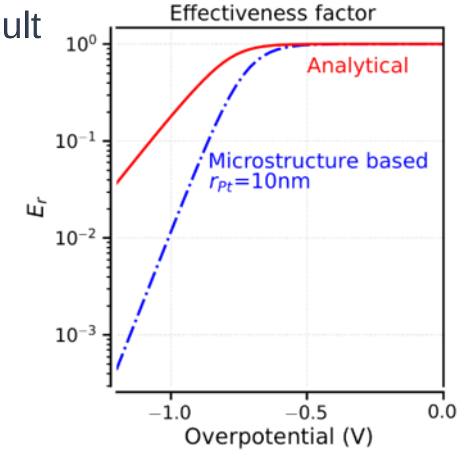
- RDE data fitted to ORR Tafel kinetics
- Two Tafel slopes observed. Slope doubling at higher overpotentials. Similar to ORR with Pt catalyst



Microscale Agglomerate Studies



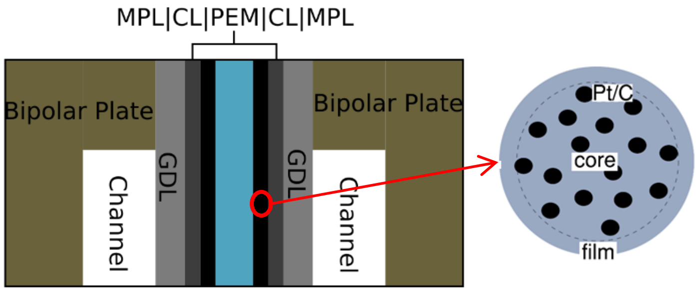
- Smaller particles result in better utilization
- Discrete catalyst particles result in lower effectiveness factor at higher overpotential (transport limited behavior)



Discreet catalyst particles result in local losses and lower catalyst utilization.

Accomplishments and Progress

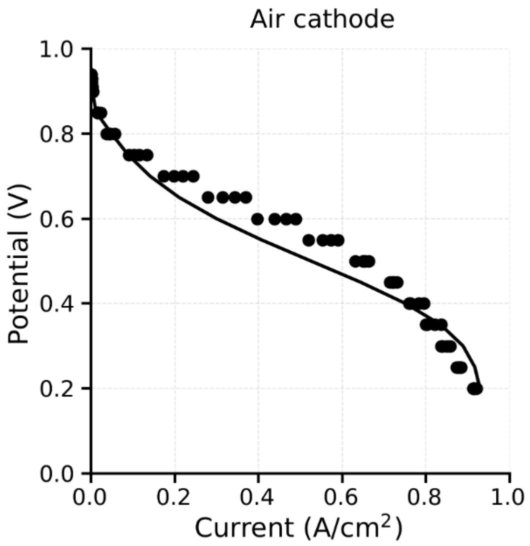
MEA level macro-scale modeling

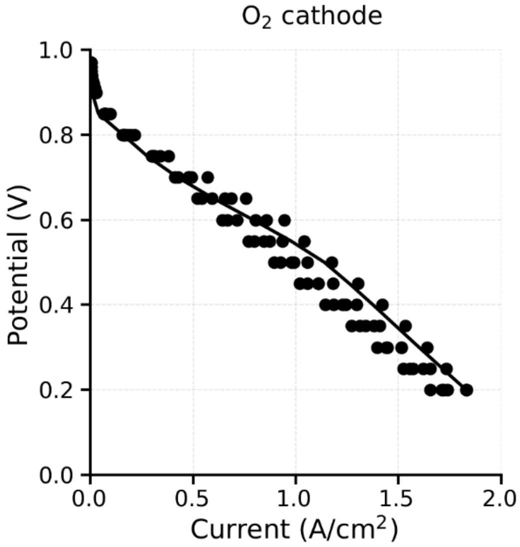


2-D cross section

2-D MEA cross-section model

- **Incorporated physics:**
  - Non-isothermal, two-phase model
  - Multicomponent diffusion
  - Electronic and protonic conduction
  - BV kinetics in anode, Dual slope Tafel in Cathode
  - Agglomerate model uses micro-scale simulated effectiveness factor





Experimental validation

- The model can predict the cell performance for various O_2 concentrations
- Dual slope kinetics predicts kinetics region accurately
- Transport limited behavior observed in air-based cathode due to lower O_2 concentrations

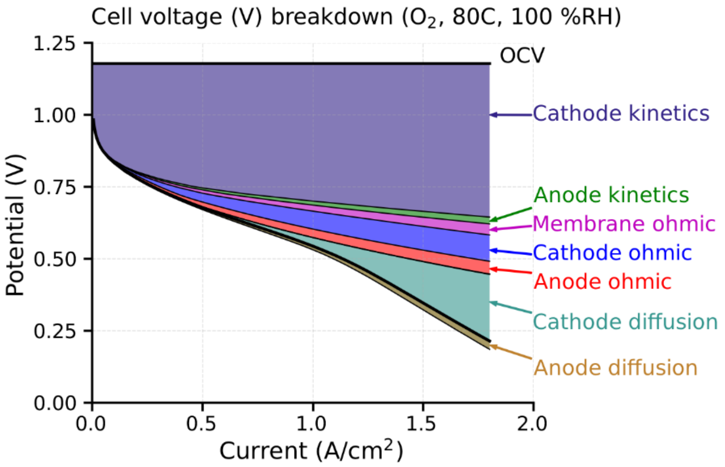
Developed predictive modeling capabilities to estimate effect of oxygen transport.

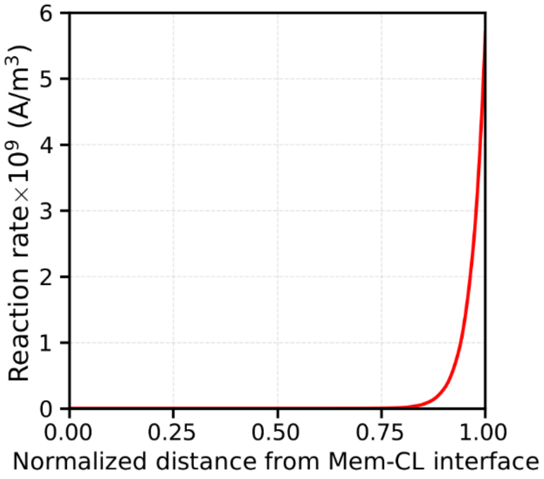
Accomplishments and Progress

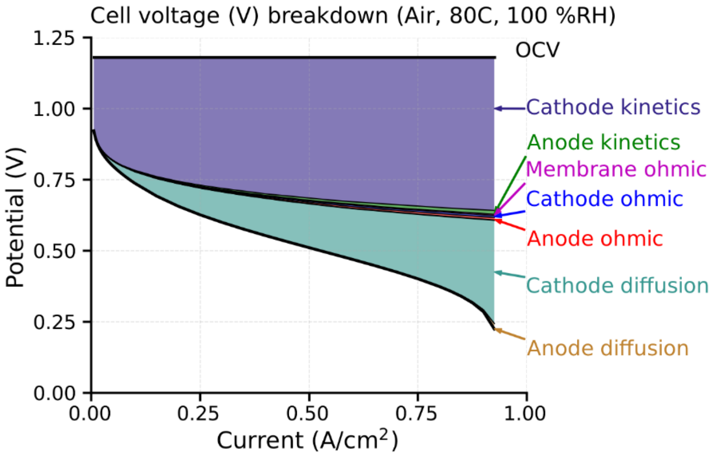
Mass transport modeling

Voltage breakdown analysis

- Significant cathode kinetics loss due to slow ORR kinetics
- Significant transport losses in cathode due to high thickness and low porosity
- Higher transport losses for lower O_2 concentration
- Higher ohmic losses in O_2 electrode due to higher cathode thickness
- Due to transport limitation, reaction is focused at CL-MPL interface
- Almost 75% of the Cathode CL is not utilized







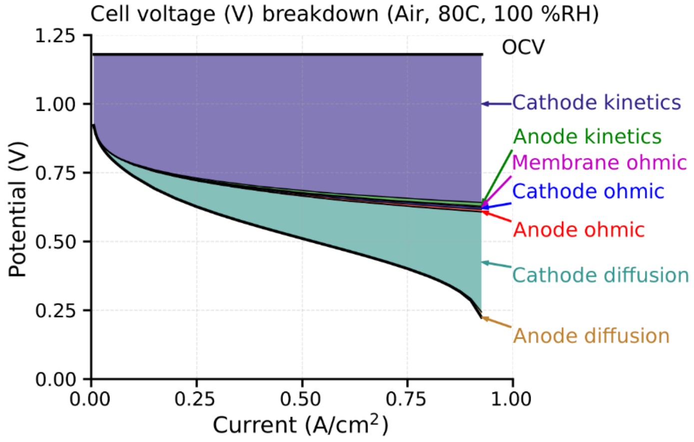
Detailed pol-curve breakdown shows limiting factors, e.g., low cCL utilization.

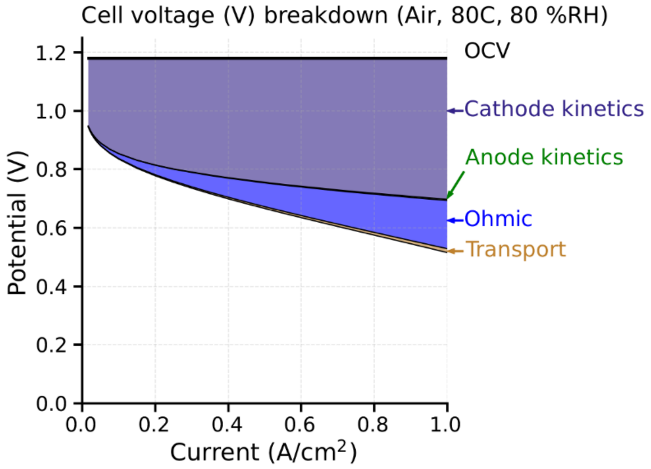
Accomplishments and Progress

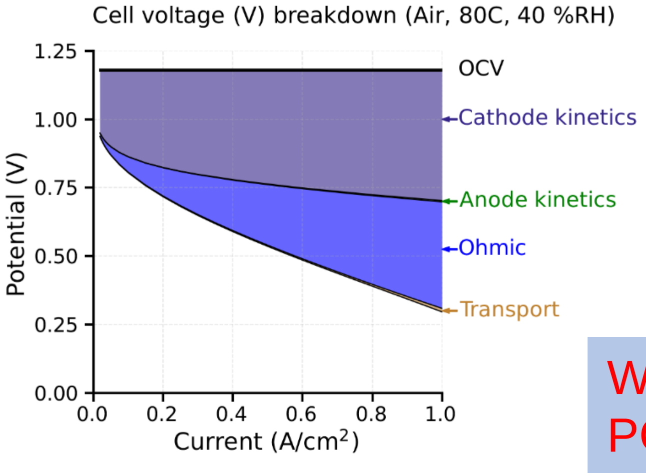
Mass transport modeling

Voltage breakdown analysis

- **Saturated conditions (100 % RH)**
  - ↳ High transport losses due to flooding
- **Higher humidity + unsaturated (80% RH)**
  - ↳ Improved performance
  - ↳ Lower transport resistance (no flooding)
  - ↳ Higher ohmic losses (lower membrane water content)
- **Low humidity, dry conditions (40% RH):**
  - ↳ Lower performance
  - ↳ Very high ohmic loss (dry membrane)
  - ↳ Transport gains not enough to compensate







Water management plays a crucial role in PGM-free catalyst-layers.

Response to Previous Year Reviewers' Comments

Several comments on the performance of the catalysts. "No MEA data were presented that would support the main expectations of this project. For that reason, all claims from the approach fall into the category of predictions and are speculative. The PIs should be acknowledged for the materials that were made and for the fact that structural characterization is consistent with what was proposed. It is not clear why these systems should be more active and durable, as well as what the foundation is for such claims." and "MEA testing is required"

- MEA evaluations in H_2-O_2 PEMFCs were conducted on the FeNC-CVD-750 catalyst, and the activity exceeded 1^{St} year Go/No-go decision point. We are still in the process of optimizing electrodes and PEMFC operation including using differential cells for the PEMFC testing. We will also work heavily on the durability testing in PEMFCs. By the end of the project, MEA-based activity and durability will be reported.

Several concerns on the activity, durability, and site density of the $M_{(x)}$-N-C catalysts such as "the potential impact would be significant if it could be demonstrated that a multi-metal active site was more active and could be reliably synthesized at high density".

- Although $Fe_{(x)}$-N-C with MMC sites was synthesized by ionothermal carbonization synthesis (slide 5), their ORR activities were not good in RDEs, and we could not improve the activities to the state-of-the-art level. We speculate that it is because either the site density is too low and/or the produced Fe_x-N_y sites are not inherently active. We decided to cease this method and focused on the CVD method because when trying to synthesize MMC sites via deposition methods, we found that the CVD method can produce highly active Fe-N-C catalysts with dense Fe-N_4 sites located exclusively on surface. Meanwhile, synthesis of MMC sites have been undergone using CVD, flash pyrolysis, and IBAD methods. One particular effort is to create N-C substrates with multiple vacancies that can host the MMC sites.

Several concerns on the collaborations "For example, it is unclear who is doing the MEA integration work, how the feedback loop from the testing is given, or how the preliminary evaluation is aligned with subsequent diagnostics." and "The value of the mass transport modeling will be apparent only if the catalyst activity becomes sufficient; otherwise, there is too much uncertainty in future catalyst morphologies that will meet activity targets"

- Although this project involves only one prime (NEU) and one sub (LBNL), productive and extensive collaborations have been undergone within these two parties, EMN Consortium Members (APS, ORNL), and unfunded partners (Giner Inc). Collaborations with APS on the in-temperature XAS revealed the Fe-N_4 site evolution pathway and led to the CVD method. Dense Fe-N_4 sites were directly visualized by STEM and EELS at ORNL. By far the PEMFC assessments reported were conducted by NEU's local partner Giner; meanwhile NEU has been learning and optimizing PEMFC testing systems and will work on the durability assessment in PEMFCs. The mass transport modeling by LBNL provided invaluable insights since NEU had a catalyst that is relatively well-defined (all Fe-N_4 sites on surface) and exhibits exceptional ORR activity in both RDE and PEMFCs for the modeling. NEU is trying to improve the catalyst from the mass transport point of view, and then on durability as well. IBAD involves collaboration between NEU and Thin-film Research inc. We will keep collaborating with EMN Consortium Members for advanced catalyst, electrode, and MEA characterizations.

Collaboration & Coordination

Northeastern University (University Prime)

Qingying Jia (PI), Sanjeev Mukerjee (Co-PI), Lynne LaRochelle Richard, Li Jiao, Qiang Sun

Catalyst design and characterizations, in situ XAS, mechanism and degradation studies, MEA fabrication and testing, management and coordination.

Lawrence Berkeley National Laboratory (National lab sub)

Adam Weber (Co-PI), Lalit Pant

Mass transport modeling

Argonne National Laboratory (EMN Consortium Member)

Deborah J. Myers, Evan Wegener, A. Jeremy Kropf

In-temperature XAS

Oak Ridge National Laboratory (EMN Consortium Member)

Dave Cullen, Karren More

STEM, EELS

Giner. Inc. (Industry unfunded partner)

Hui Xu, Fan Yang, Sichen Zhong, Thomas Stracensky

PEMFC performance and durability evaluations

Institut Charles Gerhardt Montpellier (University unfunded partner)

Frederic Jaouen, Jingkun Li, Moulay Tahar Sougrati

Mossbauer, *ex situ* XAS

Thin-films Research, Inc (Industry sub-contractor)

T.R. Raghunath

IBAD

Remaining Challenges and Barriers

- Improve the activity of Fe-N-C catalysts to reach 0.035 A·cm^{-2} and then 0.044 A·cm^{-2} at 0.9 V in H_2-O_2 PEMFCs.
- Improve the powder density of Fe-N-C catalysts to 0.5 W·cm^{-2} in a H_2-Air PEMFC.
- Improve the durability of Fe-N-C catalysts to ≤ 50% activity loss upon AST.
- Produce MMC sites with high ORR activities.
- Characterizations and Identification of MMC sites.
- Validate IBAD for the synthesis of $Fe_{(x)}$-N-C catalysts at room temperature.
- Validate flash pyrolysis for the synthesis of $Fe_{(x)}$-N-C catalysts.
- Understand the degradation modes of $M_{(x)}$-N-C catalysts and electrodes in PEMFCs.
- Scale-up of Fe-N-C catalysts made by CVD.

Proposed Future Work

- Optimize the CVD method to further improve the activity and durability of Fe-N-C catalysts.
  1. site densification (N enrichment in the N-C substrate; tune Zn-N_4 content).
  2. improve MOF-derived N-C substrate for better mass transport and durability.
  3. improve the understanding of the Fe-N4 formation mechanism in the CVD method.
- Implement IBAD to:
  1. produce $M_{(x)}$-N-C catalysts with MMC sites.
  2. realize room temperature synthesis of $M_{(x)}$-N-C catalysts.
  3. densify M-N_4 and/or MMC sites.
- Implement flash pyrolysis to improve the CVD method and to synthesize MMC sites.
- Identification of MMC sites via STEM and *in situ* XAS.
- Improve the understandings of degradation of Fe-N-C catalysts in PEMFCs via XAS studies.
- Improve the durability of $Fe_{(x)}$-N-C catalysts by:
  1. adding protective layers
  2. incorporating sacrificing oxides in N-C substrates.
  3. implementing strategies based on the new understanding of Fe-N-C degradation modes.
- Conduct IBAD and electrospinning for MEA fabrication.

- Conduct mass transport modeling to understand the bases of the activity and durability of synthesized catalysts.

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

Summary

Objective: Produce PGM-free catalysts with high ORR activity and durability in PEMFCs.

Relevance: Our approaches move beyond traditional M-N-C catalysts and synthesis routes. The new catalysts and synthesis methods may address the limited activity, durability, and active site density of $M_{(x)}$-N-C catalysts and meet the DOE targets.

Approach: $M_{(x)}$-N-C catalysts with MMC sites are targeted candidates to improve the ORR activity and durability of M-N-C catalysts. Ionothermal carbonization synthesis, non-contact pyrolysis, CVD, IBAD, and flash pyrolysis have been conducted for catalyst synthesis. Advanced characterizations are implemented to understand the catalyst formation mechanisms, ORR mechanisms, degradation mechanisms. Mass transport modeling has been implemented to understand the PEMFC performance of synthesized catalysts.

Accomplishments:

1. Fe-N_4 formation pathway during pyrolysis was revealed by in-temperature XAS.
2. CVD method was validated producing highly active Fe-N-C catalysts with all Fe-N_4 sites located on surface with 100% utilization.
3. The FeNC-CVD-750 demonstrated a current density of 0.033 $A \cdot cm^{-2}$ at 0.9 V in H_2-O_2 PEMFCs.
4. Metal deposition onto powder substrates was achieved by engineering IBAD.

Collaboration: Strong teams and effective collaborations within university (NEU), national labs (LBNL, ANL), local industry partner (Giner, Thin-Films Research), and international partner (CNRs).

Future work:

1. improve the CVD method and the flash pyrolysis.
2. implement the IBAD to synthesize $M_{(x)}$-N-C catalysts at room temperature.
3. improve the understanding of degradation of $M_{(x)}$-N-C catalysts and their durability.

Acknowledgements

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Sanjeev Mukerjee (Co-PI)
Lynne LaRochelle Richard
Li Jiao
Qiang Sun
Ershuai Liu
Serge Pann

Lawrence Berkeley National Laboratory

Adam Weber (LBNL PI),
Lalit Pant

Giner. Inc.

Hui Xu
Fan Yang
Sichen Zhong
Thomas Stracensky

Institut Charles Gerhardt Montpellier

Frederic Jaouen
Jingkun Li
Moulay-Tahar Sougrati

University of California, Los Angeles

Yu Huang, Zipeng Zhao

Thin-films Research, Inc

T.R. Raghunath

DOE Hydrogen and Fuel Cell Technologies Office (HFTO)

Nancy Garland (Technology manager)
Dimitrios Papageorgopoulos
Dave Peterson

ElectroCat
Electrocatalysis Consortium

Argonne National Laboratory

Deborah J. Myers,
Evan Wegener,
A. Jeremy Kropf
Magali S, Ferrandon
Jae Hyung Park

Oak Ridge National Laboratory

Dave Cullen, Karren More

Los Alamos National Laboratory

Piotr Zelenay, Edward F. Holby

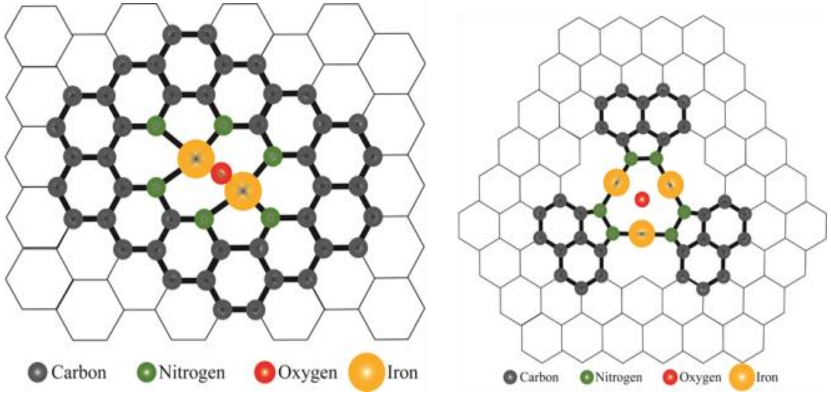
National Renewable Energy Laboratory

KC Neyerlin

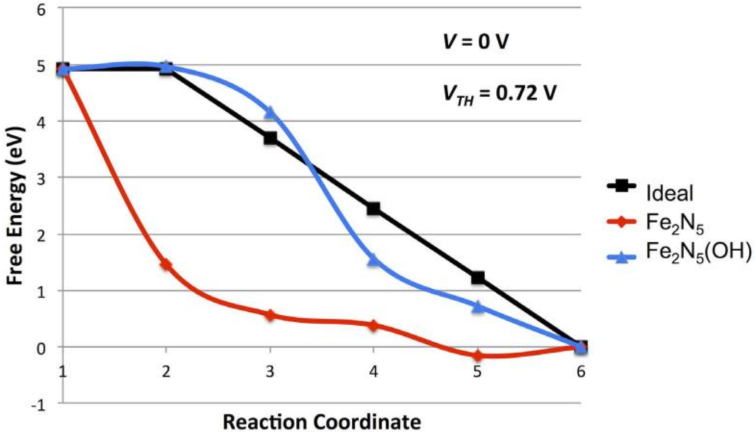
Technical Back-Up Slides

Technical Back-Up

Literature reports of the presence of MMC sites

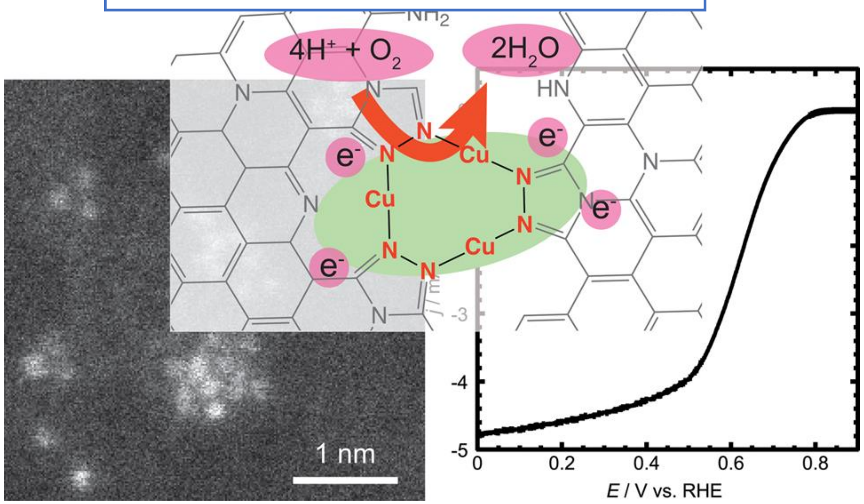


Schematic illustration of MMC sites.

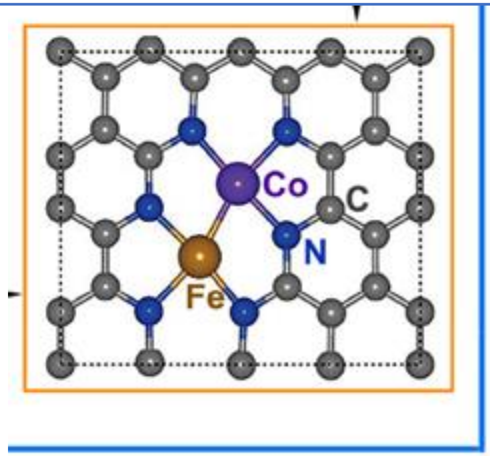


Holby, E. F.; Taylor, C. D. *Sci. Rep.* **2015**, *5*.

Desired ORR kinetics of MMC sites by DFT



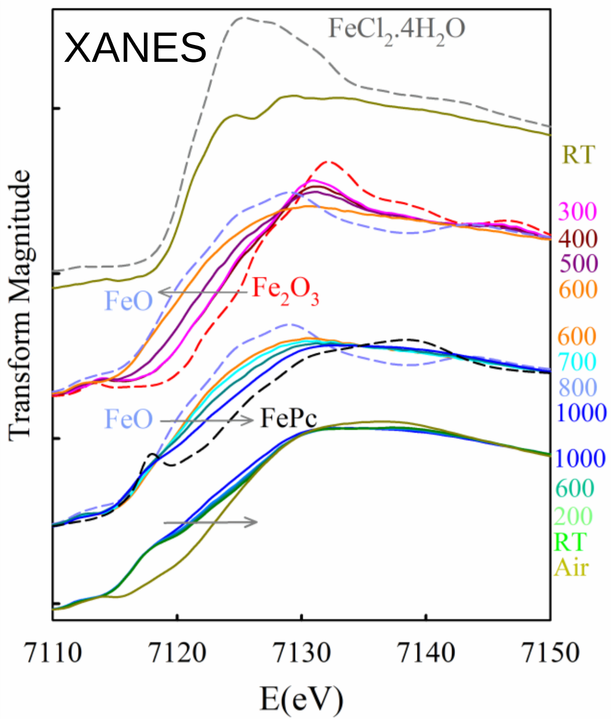
ACS Appl. Energy Mater. **2018**, 1, 2358−2364

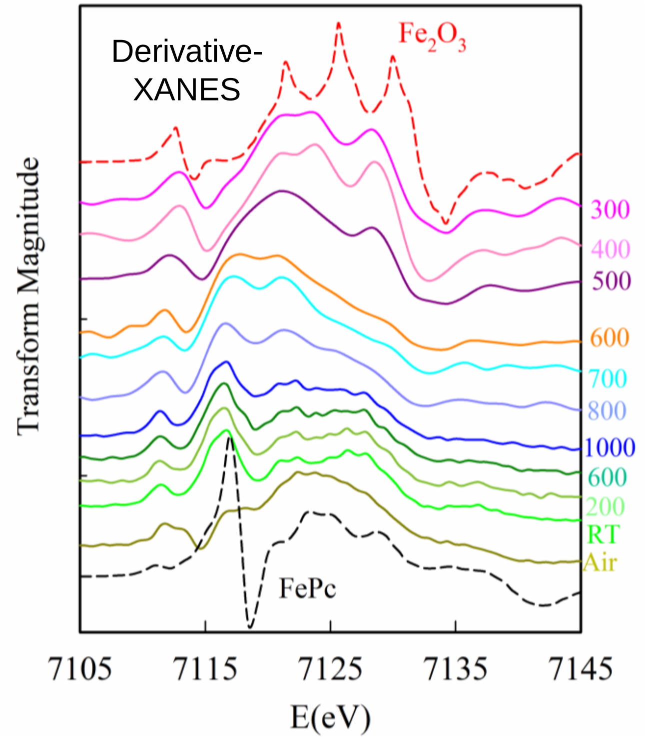


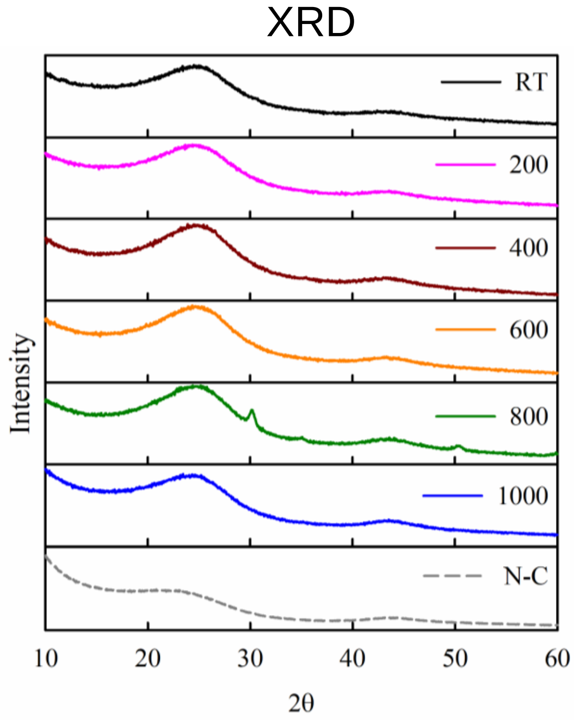
J. Am. Chem. Soc. **2017**, 139, 17281

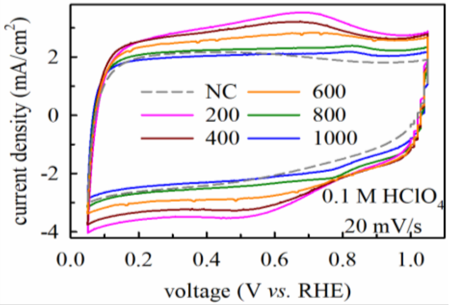
Technical Back-Up

In-temperature XAS on $FeCl_2 \cdot 4H_2O$ + N-C





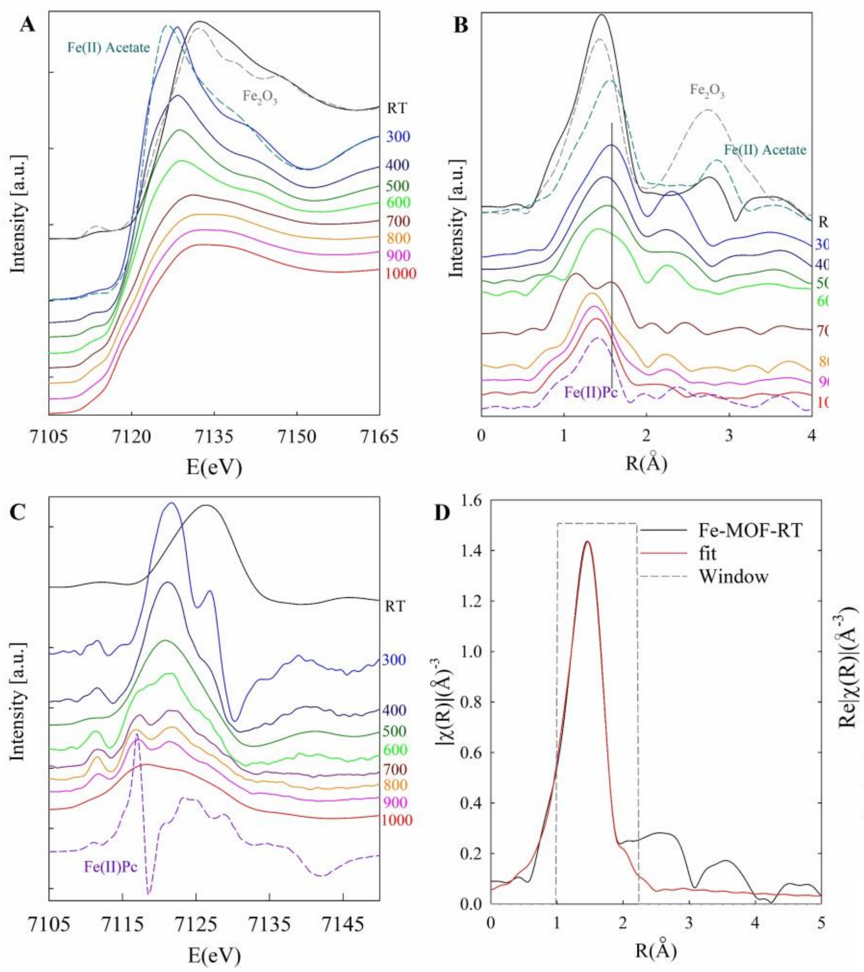




EXAFS fits	R (Å)	N	$\sigma^2 \times 10^{-3}$ (Å)	E_0 (eV)
$FeCl_2$-NC-600	1.99±0.01	3.6±0.4	17±2	-0.3±0.9
$FeCl_2$-NC-1000	1.92±0.01	4.5±0.7	12±2	-1.1 ± 1.2
$FeCl_2$-NC-RT	1.91±0.01	4.3±0.4	7±2	-0.2±1.5

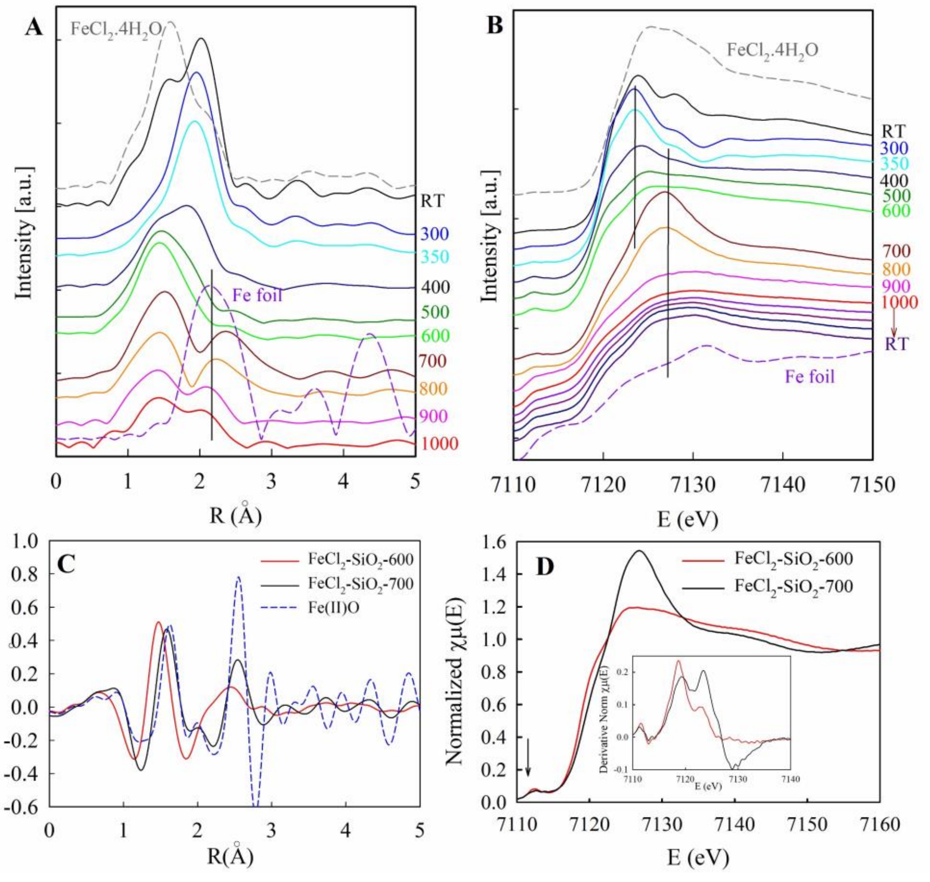
Technical Back-Up

FeAc$_2$ + ZIF-8 + Phen



	Bond	R (Å)	N	σ^2×10^{-3} (Å^2)	E$_0$ (eV)
Fe-MOF-RT	Fe-O	1.98±0.01	6.0±0.8	10±2	0.1±1.0
Fe-MOF-1000	Fe-O	1.94±0.01	3.7±0.5	13±3	-1.8±1.8

FeCl$_2$·4H$_2$O + SiO$_2$



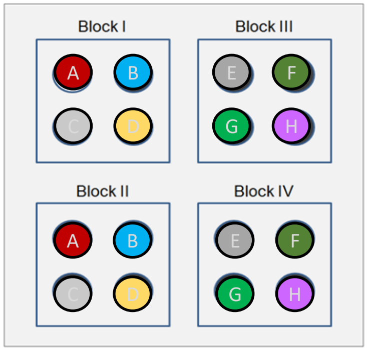
	R (Å)	N	σ^2×10^{-3} (Å^2)
FeCl$_2$-SiO$_2$-600	2.00±0.02	3.9±0.6	19±5

In-temperature XAS on other mixtures.

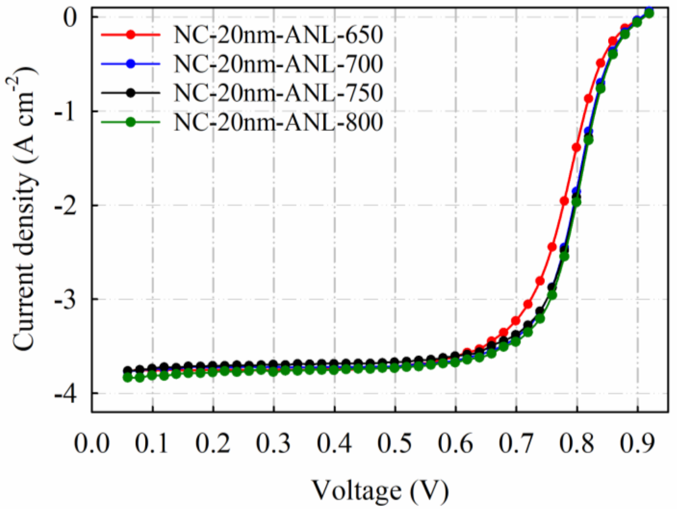
Technical Back-Up

Vertical CVD method (ANL)

HT Parallel Reactor System (T1224, Avantium)

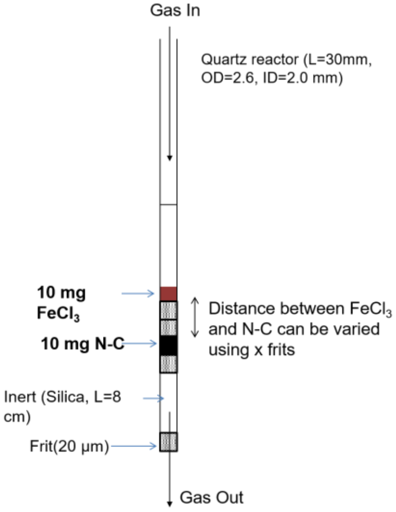


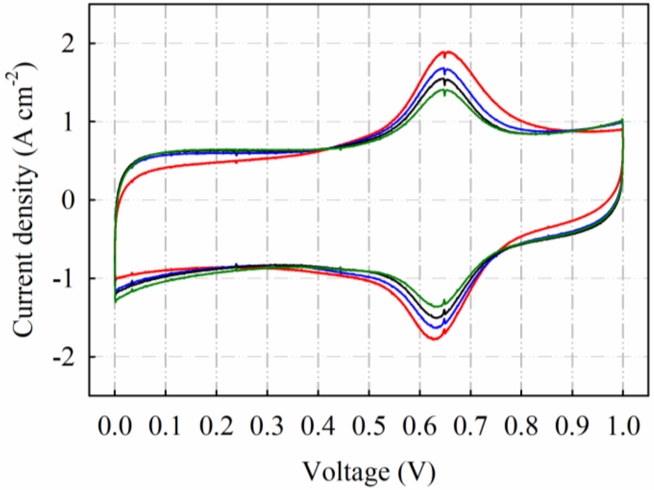
Each block can be temperature-controlled independently



Argonne NATIONAL LABORATORY

Deborah J. Myers,
Magali S, Ferrandon
Jae Hyung Park

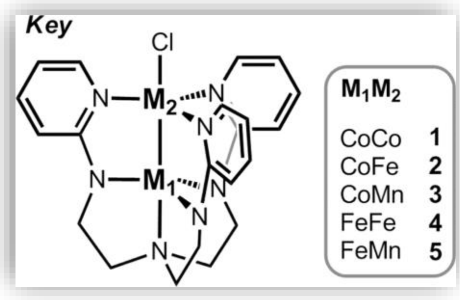




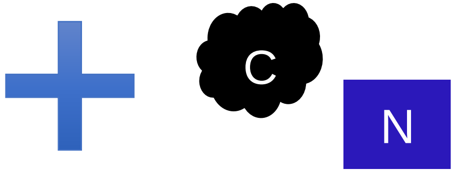
CVD was also demonstrated by another group using another system (parallel reactor).

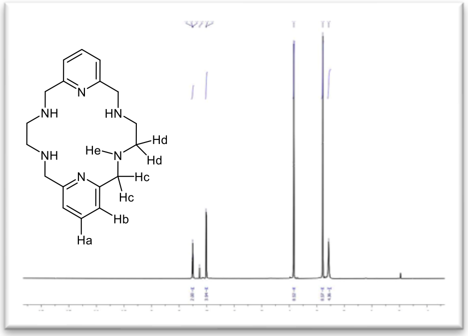
Technical Back-Up

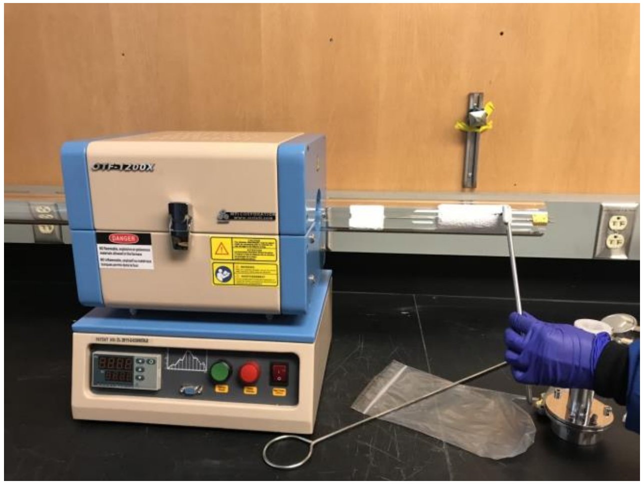
Flash pyrolysis

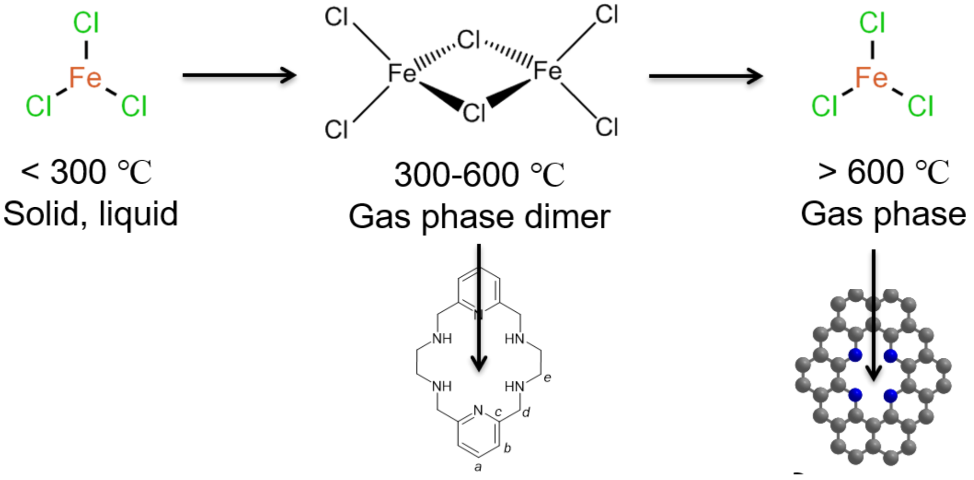


*J. Am. Chem. Soc.*2014,136,5,1842









< 300 ℃
Solid, liquid

300-600 ℃
Gas phase dimer

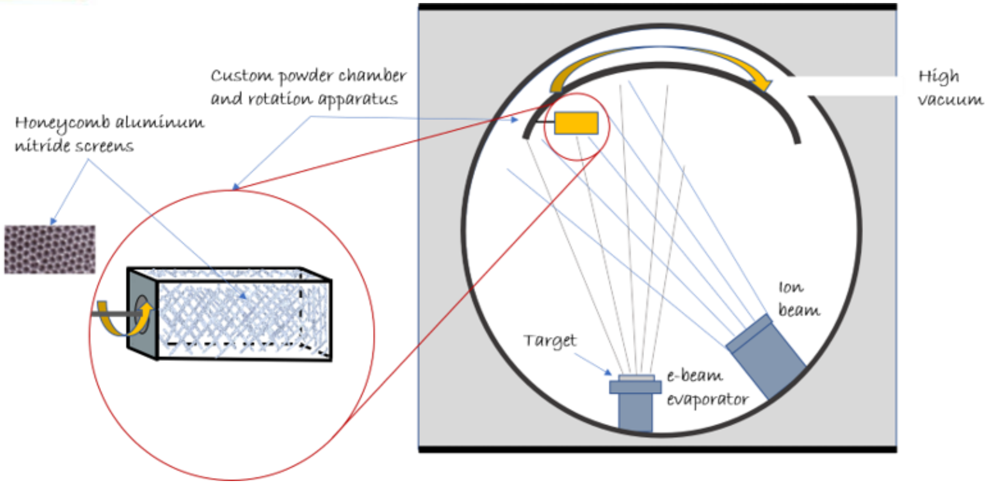
> 600 ℃
Gas phase

Synthesis of $M_{(x)}$-N-C from pre-existing MMC precursors via flash pyrolysis by a slide furnace that allows for pyrolysis at a constant temperature with controllable time.

Technical Back-Up

Engineering IBAD on powder substrates

Thin-Films Research, Inc.
270 Littleton Road
Westford MA 01886
Tel: 978-692-9530 Fax: 978-692-9531
www.thinfilmsresearch.com



- ➢ Optimized Co/N-doped precursor developed
- ➢ 9 g of optimized precursor produced for IBAD trials
- ➢ IBAD contract engineering partner identified and hired: Thin-Films Research, Inc, Westford, MA
- ➢ Tooling in late stage development and small-scale trials
- ➢ Process scalable to 5 g batches with current tool set

Publications and Presentations

Publications

- Jiao, L.; Li, J.; Richard, L.; Stracensky, T.; Liu, E.; Sun, Q.; Sougrati, Z.; Zhao, Z.; Yang, F.; Zhong, S.; Xu, H.; Mukerjee, S.; Huang, Y.; Myers, D*., Jaouen, F.,* and Jia, Q*. High-performance iron-based ORR catalysts synthesized via chemical vapor deposition. Under Preparation; Preprint available on ChemRxiv
- Li, J., Jiao, L., Wegener, E., Richard, L., Liu, E., Zitolo, A.,Sougrati, M., Mukerjee, S., Zhao, Z., Huang, Y, Kropf, A., Jaouen, F., Myers, D*., and Jia, Q*. Evolution pathway from iron compounds to Fe_1(II)-N_4 sites through gas-phase iron during pyrolysis, J. Am. Chem. Soc. 2020, 142, 1417-1423.

Conference Presentations

- Q. Jia, L. Jiao, J. Li, T. Stracensky, M. Sougrati, S. Mukerjee, F. Jaouen, D. Myers. Move beyond the evolution pathway for the formation of M-N_4 sites upon pyrolysis of the mixture of M, N, and C precursors, PRiME 2020
- Q. Jia, J. Li, D. Myers, A. J. Kropf, S. Mukerjee. Revisiting the Nature of Active Sites in Pyrolyzed Fe-N-C Electrocatalysts: In Situ Monitoring the Structure Evolution of Active Sites in Fe-N-C Catalysts during Pyrolysis. 235th ECS Meeting, 05/26/2019 **(Invited)**
- L Jiao, E Liu, LLR Richard, S Mukerjee, Q Jia. Developing Platinum Group Metal Free Catalysts with Multiple Metal Centers for the Oxygen Reduction Reaction in Acid, 235th ECS Meeting
- LLR Richard, L Jiao, E Liu, Q Jia. Development of Bimetallic Non-Platinum Group Metal Catalysts Based on Metal Organic Framework Precursors, 235th ECS Meeting
- S. Mukerjee, Q. Jia., Structural and Mechanistic Basis for the Oxygen Reduction Activity of Pyrolyzed Fe-N-C Electrocatalysts. 235th ECS Meeting

Patent

- Provisional patent: 19815-0588-INV-20028, “synthesizing highly active Fe-N-C electrocatalysts for oxygen reduction via vapor deposition of gas-phase iron”