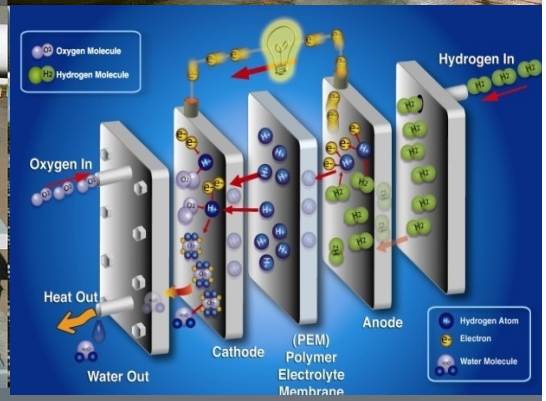
Fuel Cell Technologies Office Webinar

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy



ElectroCat and HyMARC Lab Consortia Overview

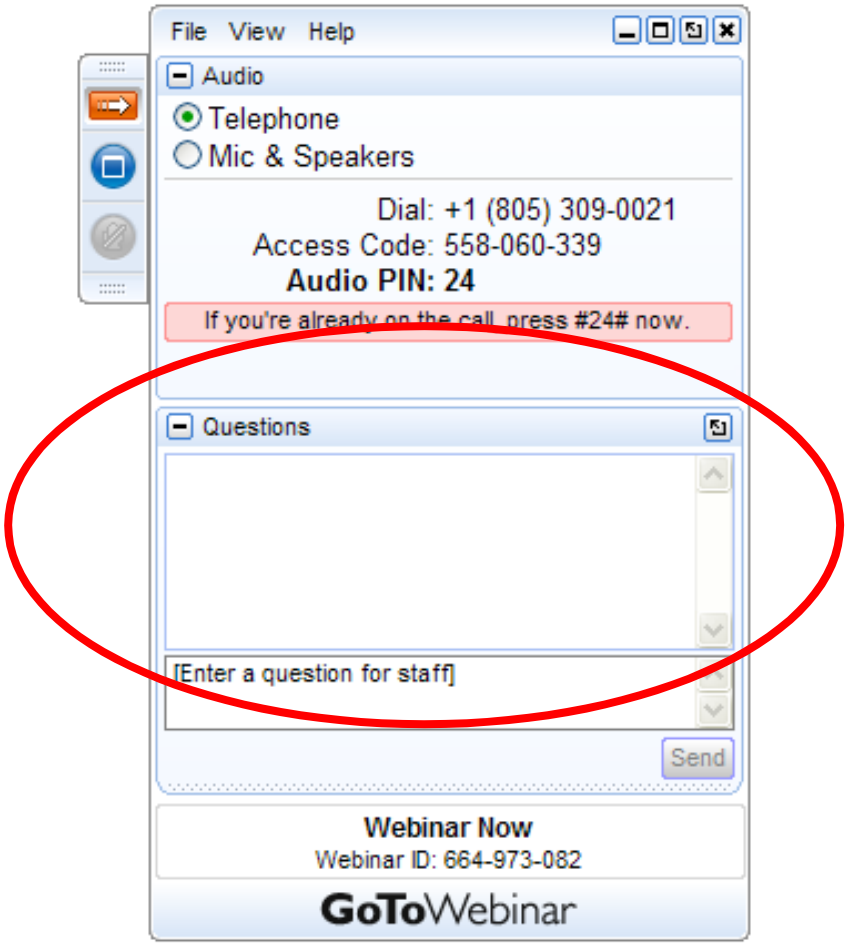
November 8, 2016

Presenter(s)

Dimitrios Papageorgopoulos, DOE-EERE-FCTO
Piotr Zelenay, Los Alamos National Laboratory
Debbie Myers, Argonne National Laboratory

Question and Answer

Please type your questions into the question box



Webinar Topics

- Summary of the organization of two Fuel Cell Technologies Office consortia within DOE-EERE's Energy Materials Network
  - Electrocatalysis Consortium (ElectroCat)
  - Hydrogen Materials—Advanced Research Consortium (HyMARC)
- Current/planned scientific activities and capabilities
- Role of individual projects selected to work with these consortia
- Utilizing existing consortia capabilities
- Upcoming FY17 Funding Opportunity Announcement (FOA)

PZ1

ElectroCat
Electrocatalysis Consortium

FCTO Lab Consortia Overview: ElectroCat

Purpose, scope, and capabilities of ElectroCat

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

November 8, 2016

Slide 4

PZ1 Minor formatting; shortened ElectroCat subheading

Piotr Zelenay, 11/4/2016

Steering Committee

Los Alamos NATIONAL LABORATORY

Piotr Zelenay

Argonne NATIONAL LABORATORY

Debbie Myers

OAK RIDGE National Laboratory

Karren More

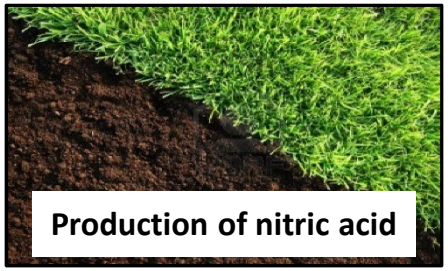
NREL NATIONAL RENEWABLE ENERGY LABORATORY

Huyen Dinh

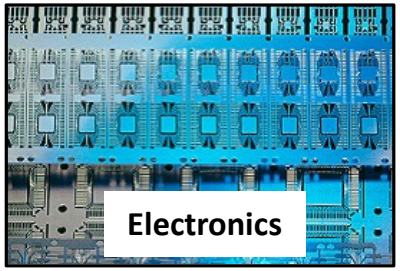
Dimitrios Papageorgopoulos and Adria Wilson, DOE-EERE-FCTO

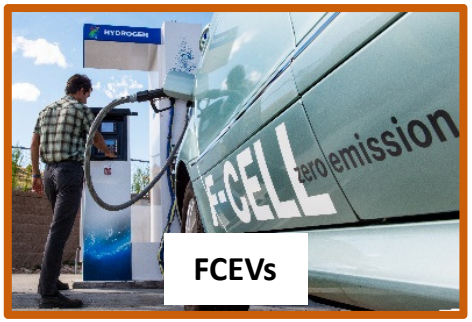
ElectroCat Materials Domain: Electrocatalysts


Petroleum refining

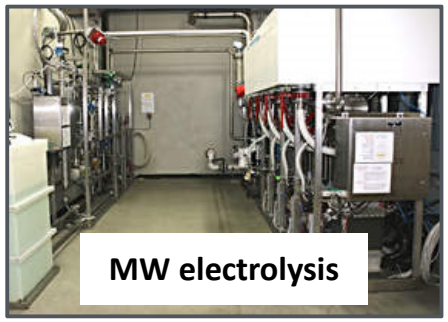

Production of nitric acid


Vehicle Pollution Control


Electronics



FCEVs

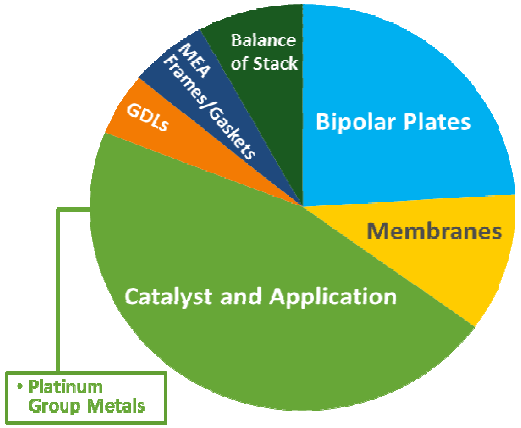

MW electrolysis

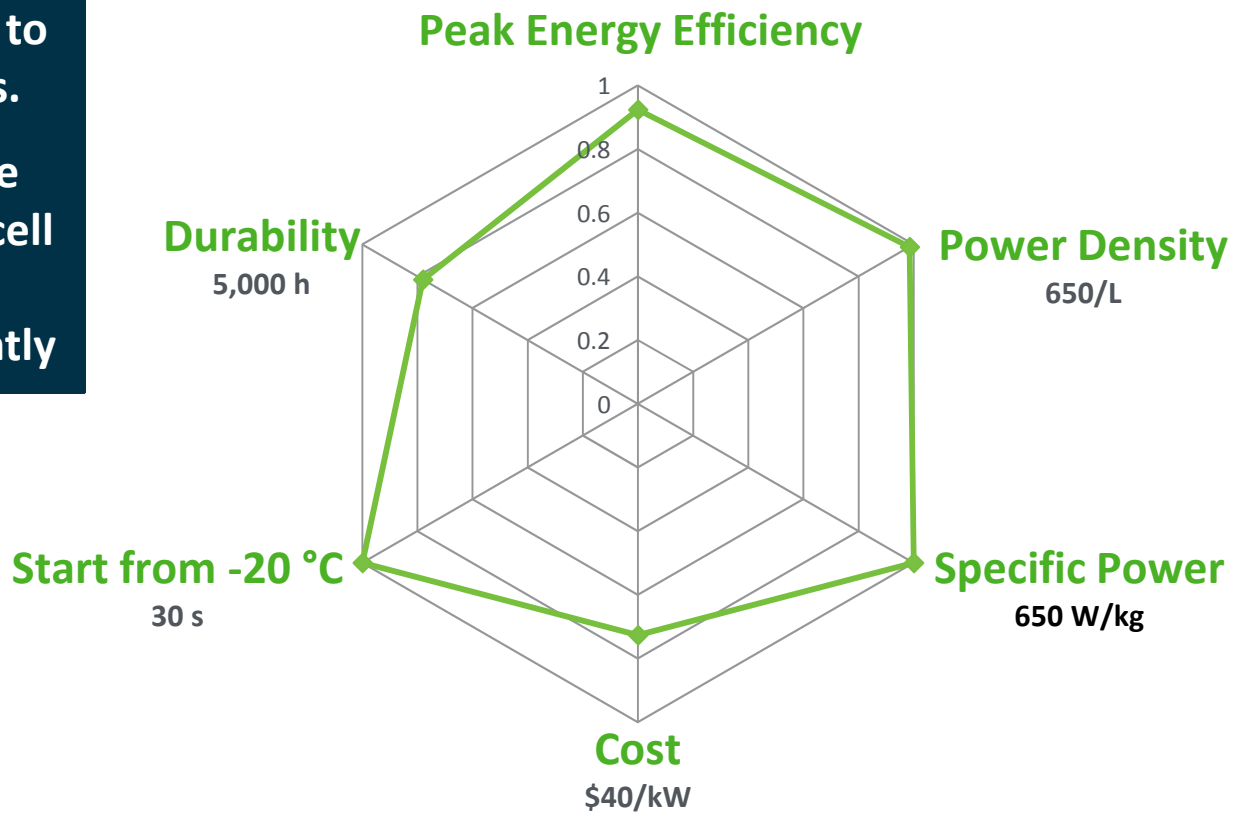
Project Focus: PGM-free catalysts for automotive fuel cells

Problem Statement

Fuel cell system targets set to be competitive with ICEVs.

Durability and cost are the primary challenges to fuel cell commercialization and must be met concurrently





PGM-free catalysts lag behind platinum in efficiency, durability, cost, and ease of integration into membrane electrode assemblies.

PGM-free *vs.* PGM Cathodes: Targeting Competitiveness

Technical Targets: Electrocatalysts for Transportation Applications			
Characteristic	**Units**	**2015 Status**	**2020 Targets**
Platinum group metal total content (both electrodes)	g/kW (rated, gross) @ 150 kPa (abs)	0.16	0.125
Platinum group metal (PGM) total loading (both electrodes)	mg_{PGM}/cm^2 (electrode area)	0.13	0.125
Mass activity	A/mg_{PGM} @ 0.9 $V_{iR\text{-}free}$	> 0.5	0.44
Loss in initial catalytic activity	% mass activity loss	66	< 40
Loss in performance at 0.8 A/cm^{2*}	mV	13	< 30
Electrocatalyst support stability	% mass activity loss	41	< 40
Loss in performance at 1.5 A/cm^2	mV	65	< 30
PGM-free catalyst activity	**A/cm^2 @ 0.9 $V_{IR\text{-}free}$**	**0.024 A/cm^2**	**> 0.044***

*Equivalent to PGM catalyst mass activity target of 0.44 A/mg_{PGM} at 0.1 mg_{PGM}/cm^2

PGM-free containing MEAs need to meet DOE performance and durability targets

Strategy: Research Priorities

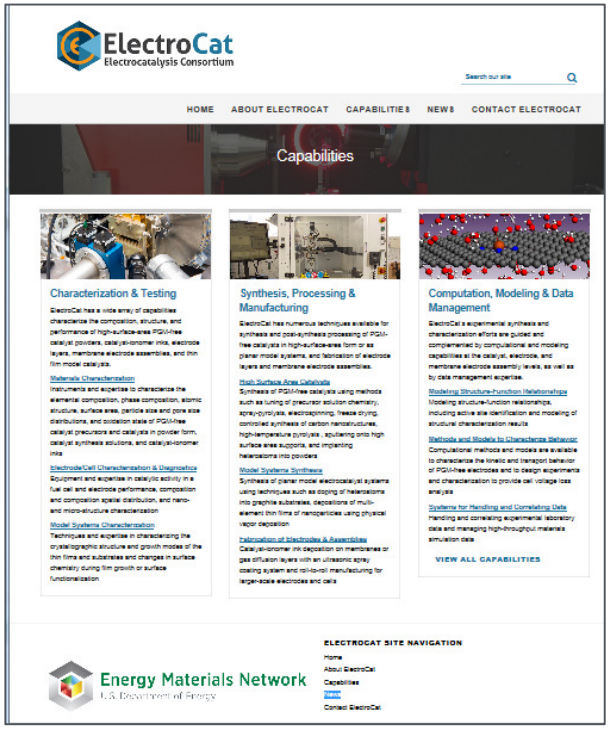
Materials Discovery & Development	**Catalysts** for oxygen reduction in low-temperature PEMFCs and PAFCs
	Catalysts for oxygen reduction and hydrogen oxidation in AMFCs
	Development of **electrodes and MEAs** that are compatible with PGM-free catalysts
Tool Development	Optimization of **atomic-scale** and **meso-scale models** of catalyst activity to predict macro-scale behavior
	High-throughput techniques for catalyst synthesis
	High-throughput techniques for characterization of catalysts, electrodes, and MEAs
	Aggregation of data in an easily searchable, public database to facilitate the development of catalyst materials and MEAs

Introduction to FOA

- High-performing and durable PGM-free catalysts and electrodes to significantly reduce fuel cell cost
- Goal is durable PGM-free oxygen reduction reaction catalysts that achieve activity of 0.044A/cm^2 at 0.9 V in a PEMFC MEA by 2020
- Proposed projects are expected to leverage specified collaboration with one or more ElectroCat national lab-based capabilities, which include:
  - catalyst synthesis, characterization, processing, and manufacturing
  - high-throughput, combinatorial techniques
  - advanced computational tools
- Projects for this topic are expected to be stage-gated with interim go/no-go decision points
- Interested applicants are encouraged to interface with the ElectroCat Steering Committee to determine potential for collaboration **before** the FOA is released

ElectroCat Capabilities Overview

http://www.electrocat.org/capabilities/



Synthesis, Processing and Manufacturing

Synthesis and post-synthesis processing of PGM-free catalysts in high-surface-area form or as planar model systems, and fabrication of electrode layers and MEAs

- ✓ High surface area catalysts
- ✓ Model systems synthesis
- ✓ Fabrication of electrodes and membrane-electrode assemblies

Characterization and Testing

Composition, structure, and performance of high-surface-area PGM-free catalyst powders, catalyst-ionomer inks, electrode layers, membrane electrode assemblies, and thin film model catalysts.

- ✓ Materials Characterization
- ✓ Electrode/Cell Characterization & Diagnostics
- ✓ Model Systems Characterization

Computation, Modeling and Data Management

Guiding and complementing experimental efforts with computational and modeling capabilities at the catalyst, electrode, and membrane electrode assembly levels, as well as by data management expertise.

- ✓ Modeling structure-function relationships
- ✓ Methods and models to characterize behavior
- ✓ Systems for handling and correlating data

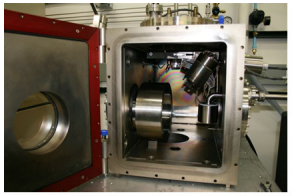
Synthesis, Processing and Manufacturing Capabilities

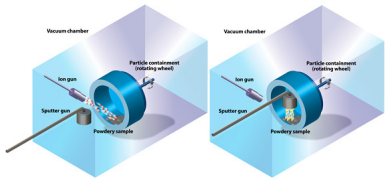
High Surface Area Catalysts

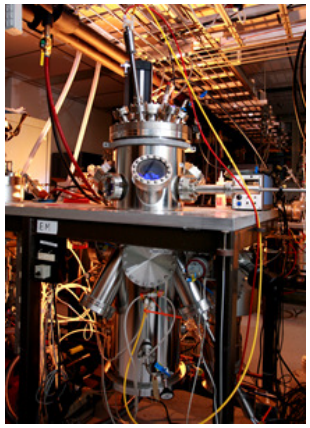
- PGM-free Catalyst Synthesis, Analytical Characterization, and Electrochemical and Fuel Cell Testing (LANL)
- Sputter Deposition of Thin Films and High Surface Area Catalysts (ORNL)
- Powder Sputter and Implant System (NREL)
- High-throughput Synthesis of PGM-free Catalysts and Electrodes (ANL)

Model Systems Synthesis

- Controlled Functionalization of Model Catalysts (LANL)
- Sputter Deposition of Thin Films and High Surface Area Catalysts (ORNL)
- High-throughput (HT) Thin Film Fabrication and Characterization (NREL)

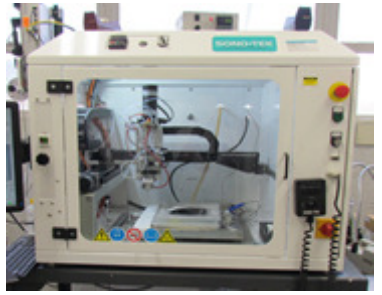






Fuel Cell Fabrication

- Membrane-Electrode Assembly Fabrication (LANL)
- High-throughput Synthesis of PGM-free Catalysts and Electrodes (ANL)
- High-throughput Approaches to Scaling PGM-free Electrodes (NREL)
- Manufacturing Porous Electrodes (ORNL)



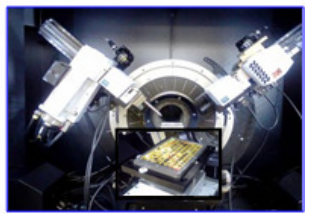
Characterization and Testing Capabilities

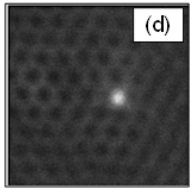
Materials Characterization

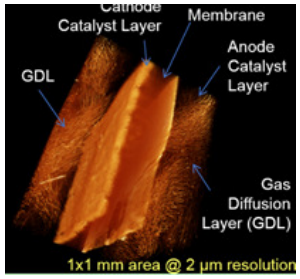
- PGM-free Catalyst Synthesis, Analytical Characterization, and Electrochemical and Fuel Cell Testing (LANL)
- X-Ray Characterization Techniques (LANL)
- X-Ray Photoelectron Spectroscopy (ORNL)
- Electron Tomography (ORNL)
- Analytical Electron Microscopy (ORNL)
- In situ Electron Microscopy (ORNL)
- Structure/Composition-Function Relationships and Active Sites (ANL)
- In situ and Operando Atomic, Nano-, and Micro-structure Characterization (ANL)
- Combinatorial Hydrodynamic Screening of PGM-free Catalyst Activity and Stability (ANL)
- High-throughput Characterization of PGM-free Catalysts and Electrodes (ANL)

Electrode and Cell Characterization

- Operando Differential Cell Measurements of Electrochemical Kinetics and Transport (NREL)
- PGM-free Catalyst Synthesis, Analytical Characterization, and Electrochemical and Fuel Cell Testing (LANL)
- Electrode Microstructure Characterization and Simulation (ANL)
- Electron Tomography (ORNL)
- Analytical Electron Microscopy (ORNL)
- In situ and Operando Atomic, Nano-, and Micro-structure Characterization (ANL)
- Segmented Cell System Optimized for R&D Combinatorial Studies (NREL)
- In situ Fluoride and Carbon Dioxide Emission Measurements (LANL)
- Segmented Cell and Neutron Imaging (LANL)
- High-throughput Characterization of PGM-free Catalysts and Electrodes (ANL)







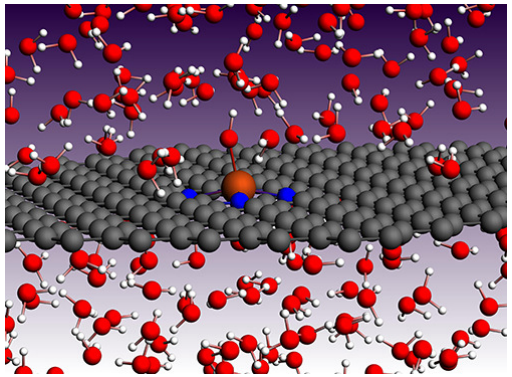
Model Systems Characterization

- Controlled Functionalization of Model Catalysts (LANL)
- X-Ray Photoelectron Spectroscopy (ORNL)
- High-throughput (HT) Thin Film Fabrication and Characterization (NREL)

Computation, Modeling & Data Management

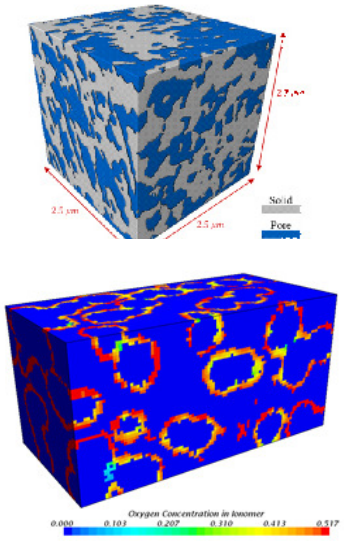
Catalyst Modeling

- Multi-scale Modeling
- Rational Design of PGM-free Catalysts (LANL)



Electrode/Fuel Cell Performance Modeling

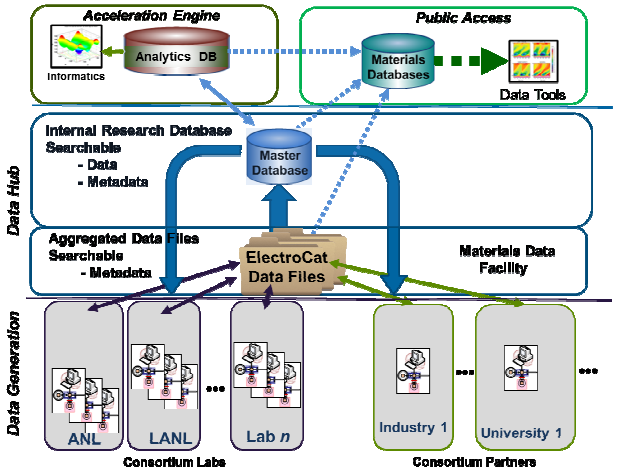
- Electrode Microstructure Characterization and Simulation (ANL)
- Modeling Kinetic and Transport Processes in PGM-free Electrodes (ANL)



Oxygen transport

Data Management

- Experimental and Computational Materials Data Infrastructure (NREL)
- Materials Data Facility and Globus (ANL)



Capability Navigation

Materials Characterization

PGM-free Catalyst Synthesis, Analytical Characterization, and Electrochemical and Fuel Cell Testing

The expertise in PGM-free catalyst synthesis, characterization, and fuel cell testing at LANL is built on decades-long experience and proven results, and is the most important capability within LANL's PGM-free program by far.

ELECTRODE/CELL CHARACTERIZATION | HIGH SURFACE AREA CATALYSTS | MATERIALS CHARACTERIZATION | SYNTHESIS/PROCESSING/MANUFACTURING

All Capabilities

Characterization & Testing

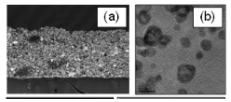
>> *Materials Characterization*

>> *Electrode/Cell Characterization & Diagnostics*

>> *Model Systems Characterization*

Analytical Electron Microscopy

Laboratory:	Oak Ridge National Laboratory (ORNL)
Capability Expert:	Karren L. More
Capability Details:	
Title:	High-resolution analytical scanning transmission electron microscopy (STEM)
Class:	Characterization
Description:	High-resolution transmission electron microscopy (TEM) and aberration-corrected scanning transmission electron microscopy (STEM) are microscopy methods used to characterize the atomic-scale structure of PGM-free catalysts (typically in powder form) and the material constituents (catalyst and ionomer) comprising membrane electrode assemblies (MEAs). STEM instruments are typically equipped with multiple detectors, including high angle annular dark field (HAADF) detectors to perform what is commonly referred to as Z-contrast STEM imaging (where Z refers to the atomic number), bright field (BF) detectors, and spectrometers (e.g., an electron energy loss spectrometer (EELS) and an energy dispersive X-ray spectrometer (EDS)). These detectors and spectrometers, when used in combination, enable the simultaneous study of the atomic structure and chemistry of novel PGM-free catalyst systems and their interfaces with other MEA constituents from the bulk-scale to the single atom level. Compositions and chemistries can be acquired and mapped (spectral imaging) across multiple length scales and directly correlated with the atomic structure determined through HAADF/BF-STEM imaging.
Capability Bounds:	NA
Unique Aspects:	A full suite of scanning transmission electron microscopes (STEM) is available at ORNL for conducting imaging and spectroscopic analysis of PGM-free catalysts and membrane electrode assemblies (MEAs) from the bulk-scale to the single-atom level, including the identification of unique morphologies of catalyst particles and insight towards understanding the atomic structure of catalytically active sites. Unique microscopes include low-voltage (60kV) and high-voltage (200kV) aberration-corrected STEM instruments equipped with high-energy resolution electron energy loss spectroscopy (EELS) and high spatial-resolution energy dispersive X-ray spectroscopy (EDS), which enable a broad range of structural, chemical, and
Availability:	Instruments in ORNL's Materials Characterization Center (MCC) are available for partnership with industry through Strategic Partnership Projects (SPP), cooperative research and development agreements (CRADAs) via full-cost recovery (hourly fee), and direct project collaborations to facilitate new materials discovery and understanding; instruments in ORNL's Center for Nanophase Materials Sciences (CNMS – a U.S. DOE Office of Science User Facility) are accessible through a peer-reviewed proposal process (no cost if results are publishable and full-cost recovery if data is proprietary). All instruments in the MCC and CNMS are available for characterization of PGM-free catalysts and MEAs.
References:	G. Wu, K.L. More, C.M. Johnston, and P. Zelenay, "High-Performance Electrocatalysts for Oxygen Reduction Derived from Polyanilene, Iron, and Cobalt," *Science* 332 443-447 (2011). W. Gao, G. Wu, M.T. Janicke, D.A. Cullen, R. Mukundan, J.K. Baldwin, E.L. Brosha, C. Garlande, P.M. Ajayan, K.L. More, A.M. Dattlebaum, and P. Zelenay, "Ozonated Graphene Oxide Film as a Proton Exchange Membrane," *Angewandte Chemie International Edition* 53 [14] 3588-3593 (2014). G. Wu, K.L. More, P. Xu, H.L. Wang, M. Ferrandon, A.J. Kropf, D.J. Myers, S. Ma, C.M. Johnston, and P. Zelenay, "A Carbon-nanotube-supported Graphene-rich Non-precious Metal Oxygen Reduction Catalyst with Enhanced Performance Durability," *Chemical Communications* 49 3291-3293 (2013).
Benefit:	ORNL's unique STEM instruments provide capabilities for the complete analytical and structural characterization of PGM-free catalysts and MEAs at multiple length scales to correlate structure and chemistry with material performance.



Title

Laboratory: **LANL, ANL, ORNL, or NREL**

Capability Expert: *Person to contact with specific questions about capability*

Capability Details:

- **Title**
- **Class**
- **Description**
- **Capability Bounds**
- **Unique Aspects**
- **Availability**
- **References**
- **Benefit**
- **Illustrative Graphic**

- **Questions about capabilities:**

  Contact@ElectroCat.org

  (to Steering Committee members)

- **Questions about FOA:**

  http://energy.gov/eere/fuelcells/subscribe-news-and-financial-opportunity-updates

- **Note:** If you intend to interact with ElectroCat through a FOA-awarded project, please do not contact either Steering Committee members or capability experts after the FOA has been released

Thank you

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