ElectroCat Lab Consortium Overview

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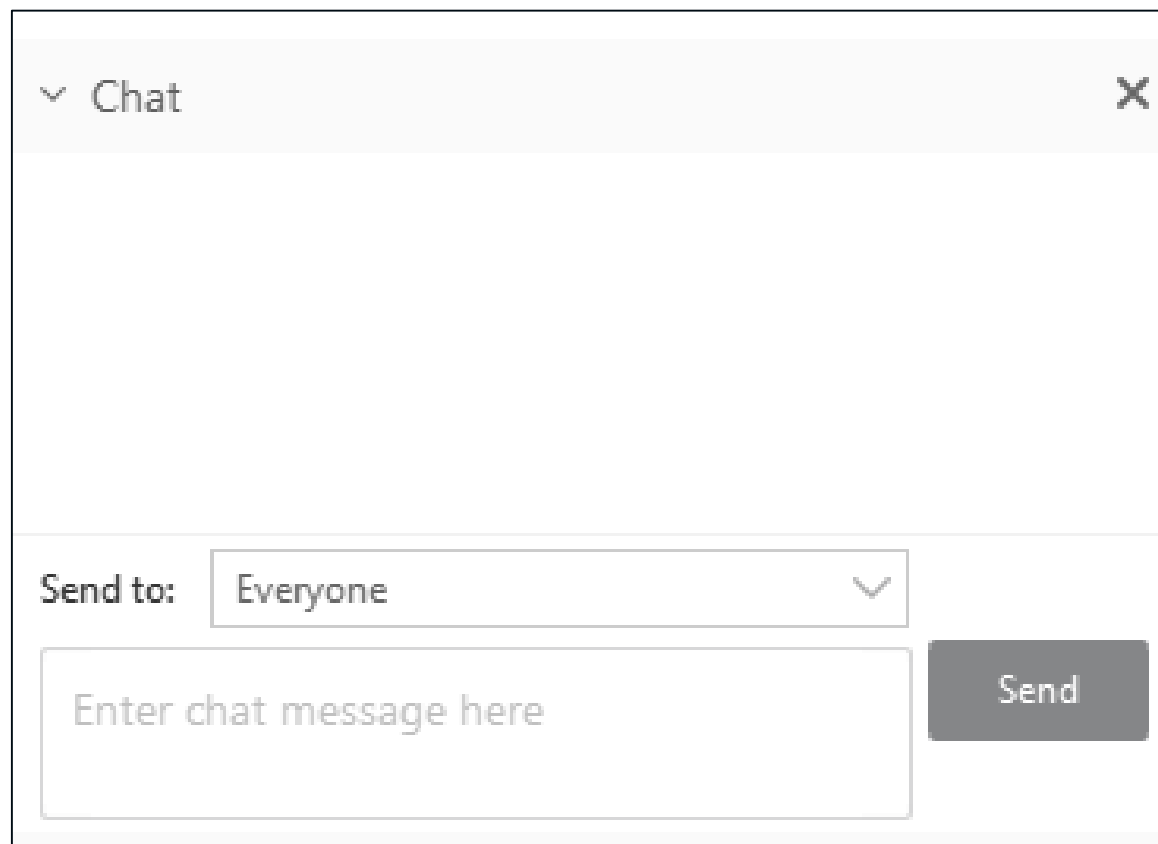
Fuel Cell Technologies Office Webinar

April 30, 2018

Question and Answer

Please type your questions into
the question box. **Send to HOST**

Webinar Topics

- Summary of the organization of ElectroCat

- Current/planned scientific activities and capabilities

- Role of individual projects selected to work with this consortium

- Utilizing existing consortium capabilities

- Fuel Cell Technologies Office (FCTO) FY18 Funding Opportunity Announcement (FOA)

Steering Committee

Los Alamos NATIONAL LABORATORY

Piotr Zelenay

Argonne NATIONAL LABORATORY

Debbie Myers

OAK RIDGE National Laboratory
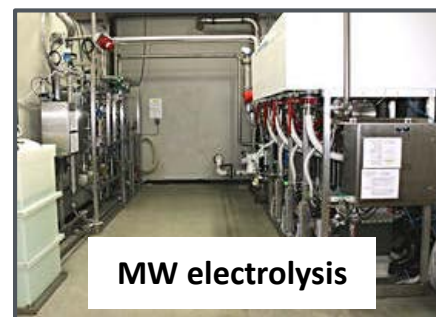
Karren More

NREL NATIONAL RENEWABLE ENERGY LABORATORY

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ElectroCat Electrocatalysis Consortium

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ElectroCat Materials Domain: Electrocatalysts

Petroleum refining

Production of nitric acid

Vehicle Pollution Control

Electronics

FCEVs

MW electrolysis
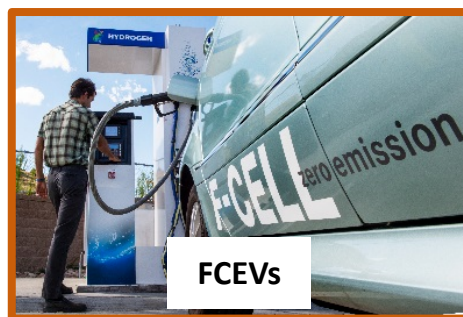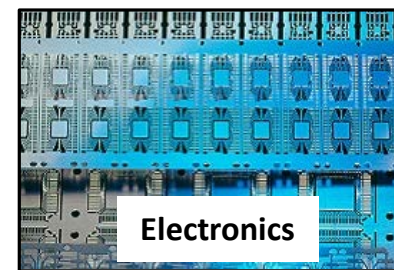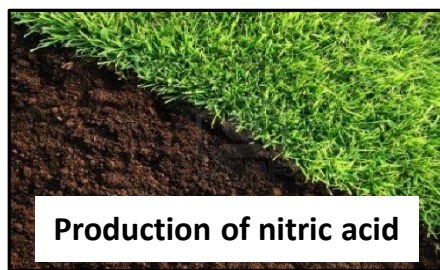
Project Focus: PGM-free catalysts for automotive fuel cells

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

Technical Targets: Electrocatalysts for Transportation Applications			
Characteristic	**Units**	**2018 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

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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

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Introduction to FOA

- Early-stage R&D for 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 0.044 A/cm^2 at 0.9 V in a PEMFC MEA by 2025

- 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

ElectroCat Capabilities Overview
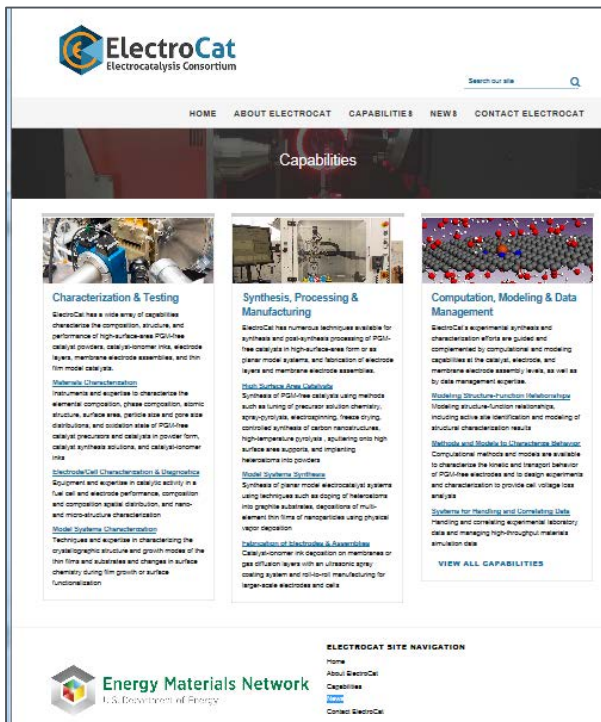
Synthesis, Processing and Manufacturing

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

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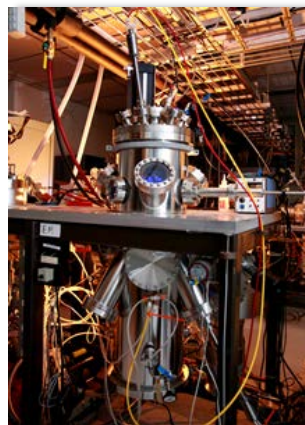# Synthesis, Processing and Manufacturing Capabilities

High Surface Area Catalysts

- PGM-free Catalyst Synthesis, Analytical Characterization, and Electrochemical and Fuel Cell Testing (LANL)
- High-throughput Synthesis of PGM-free Catalysts and Electrodes (ANL)

Model Systems Synthesis

- Controlled Functionalization of Model Catalysts (LANL)

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)

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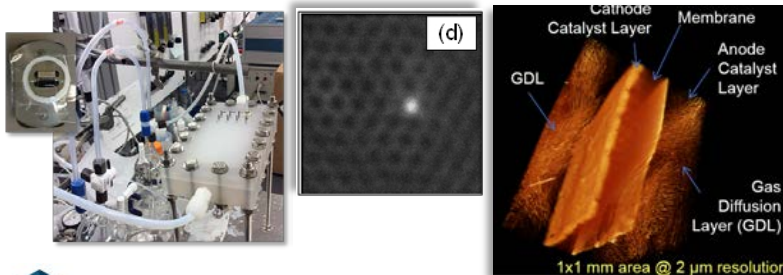# Characterization and Testing Capabilities

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)
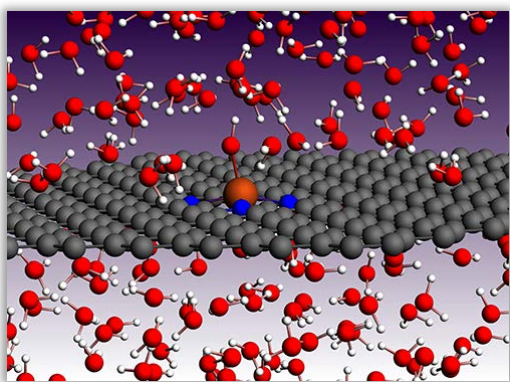
Model Systems Characterization

- Controlled Functionalization of Model Catalysts (LANL)
- X-Ray Photoelectron Spectroscopy (ORNL)

Cathode Catalyst Layer
Membrane
Anode Catalyst Layer
GDL
Gas Diffusion Layer (GDL)
(d)
1x1 mm area @ 2 μm resolution

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Computation, Modeling & Data Management
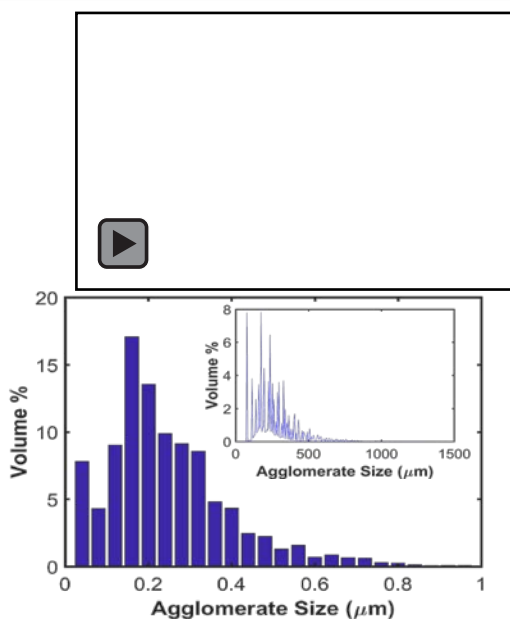
Catalyst Modeling

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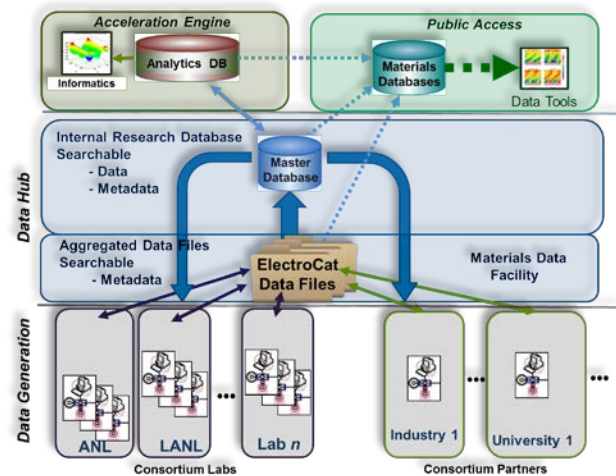

Electrode/Fuel Cell Performance Modeling

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

Data Management

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

https://datahub.electrocat.org

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

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

Analytical Electron Microscopy

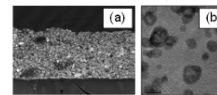| Laboratory: | Oak Ridge National Laboratory (ORNL) |
Capability Expert:	Karren L. More
Capability Details:	
Title:	High-resolution analytical scanning transmission electron microscopy (STEM)
Class:	Characterization
Description:	High-resolution transmission electron microscopy (TEM) and aberration-corrected 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 Polyaniline, 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.

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Application

- **Apply to the FOA:**

  https://eere-exchange.energy.gov/#FoaId79690f66-6dc9-47e9-ac9f-86057538ae44

- **Questions about capabilities:**

  Contact@ElectroCat.org

- **Questions about FOA:** All questions pertaining to this funding opportunity announcement should be emailed to FCTOFOA@ee.doe.gov

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

Thank you

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www.hydrogenandfuelcells.energy.gov

www.electrocat.org/capabilities/