Breakout Group 1: Catalysts and Supports

PARTICIPANTS

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GAPS/BARRIERS

- Need a 4x improvement in oxygen reduction reaction (ORR) kinetics

Lack of:

- Understanding biomimetic catalysts and their potential for fuel cell application
- Fundamental understanding
  - of active sites in non-platinum group metal (PGM) catalysts
  - of active sites in PGM catalysts
  - of catalyst-support interaction
- Coordination of molecular modeling with synthesis and testing
- Rational design of catalysts and catalyst/support systems based on fundamental understanding of active sites and reaction mechanisms
- Stable supports and active catalysts
- Anode catalysts that are not active for ORR to prevent high cathode potentials during start-up/shut-down
- Supports that maximize mass transport to non-PGM catalysts
- Preparation methods that lead to stable and active catalysts
- Anode catalysts for direct low-temperature oxidation of liquid fuels
- Fundamental studies of operating fuel cells
- Accelerated testing that reflects real-world operating conditions

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RD&D NEEDS
(priority votes are shown in parentheses)

FUNDAMENTAL UNDERSTANDING & DETAILED CHARACTERIZATION	CATALYST/SUPPORT DEVELOPMENT	ANODE CATALYSTS FOR ALTERNATIVE FUELS

• Fundamental studies to understand catalyst morphology, size, and composition combined with catalyst-support interactions at the nanometer-scale **(8)**
• Current catalysts relative to transportation
  - Studies of catalytic activity at the active site
  - Transport of protons and electrons to/from active site in the ionomer environment
• Analysis/characterization of catalysts before, during, and after fuel cell testing
  - Composition, particle size, crystal structure, morphology, dispersion
  - Nanostructured catalysts and supports for core-shell systems and non-PGM systems, e.g., NEXAFS of adsorbates on core-shell and skin model surfaces
• Accessibility of platinum (Pt) in catalyst layer
  - Supports that enhance catalytic and transport functions
  - Binders that enable greater access to catalyst sites
• Fundamental *in situ* studies of effect of support properties on catalyst stability
  - Carbon supports
  - Non-carbon supports
• Understanding activity-composition-structure relationships for ORR catalysts
• Understanding catalyst layer structures
  - Effect of pore distribution
  - Effect of interaction with ionomer
  - Effect of mass transport
• Modeling catalyst/support layers and validation of mechanistic models with experiment
• Modeling and testing of catalyst dynamics (transport & kinetics)
	• New catalysts
	  - Low-Pt: core shell, structure-controlled
	  - Non-PGM **(7)**
	  - Biomimetic
	• Physicochemical properties of supports that enhance stability of the catalyst/support system
	• Novel synthetic effort
	  - Detailed structural studies
	  - Integrated theory and modeling with synthesis
	  - Integrated team effort in theory, synthesis, and testing in fuel cell environment
	• Development of hydrogen oxidation catalysts with low ORR activity
	• Development of viable supports that would allow increase in loading (thickness) for non-PGM catalysts
	• New techniques/tools to couple experiment with molecular modeling to test predicted performance improvement
		• Multi-metal alloys
		  - Activity determination
		  - Corrosion resistance
		• *In situ* studies of catalyst degradation mechanisms
		  - Effect of interaction with carbon support
		  - Effect of catalyst particle size
		  - Effect of catalyst structure

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RD&D NEEDS (Cont'd)
(priority votes are shown in parentheses)

DURABILITY & ACCELERATED TESTING	PROJECT IMPLEMENTATION	OTHER

• *In situ* studies of catalyst degradation mechanisms **(9)**
  - Effect of interaction with carbon support
  - Effect of Pt particle size
  - Effect of Pt structure
• Understanding of morphology/physical characteristics of catalysts on durability
• Fundamental studies of catalyst degradation under automotive duty cycles/stresses
  - Definition of appropriate stress conditions
  - Carbon corrosion
  - Pt dissolution
• Understanding relationships between catalysts and impurities
  - Characterize impurity impact on catalyst performance and durability
	• Teaming arrangements encouraged
	  - Industry
	  - Universities
	  - National laboratories
	• "Standard" catalyst samples
	• Standard test protocols
	  - Universal testing protocol for catalyst activity studies
		• Explore procedures for catalyst/MEA preparation together with detailed characterization (porosity, SA, etc.) and performance measurements
		  - Understand the effects of preparation procedures on performance and life.
		• Effect of Pt price on DOE targets
		• Sensors for low concentrations of hydrogen in pure oxygen at 100% relative humidity
		• Sensors for low concentrations of oxygen in pure hydrogen at 100% relative humidity
		• Sensors operational at up to 1,200 psi and 90°C