

# Electrocatalysis Breakout Session

# Anode

ANODE (H<sub>2</sub>//O<sub>2</sub>/Air)

## 1. *Fundamental understanding of HOR on Pt and candidate non-PGM catalysts*

- Discussion of possible role of specific adsorption of hydroxide
- Discussion of role of local mobility of OH<sup>-</sup> in the anode double layer
- Role of active site in non-PGMs.
- Flooding – ionomer/catalyst
- Role of CO<sub>2</sub> as a poison based on electro-migration (carbonate species crossover and its eventual reduction).
- Role of oxygen crossover in the context of anode Electrocatalysis
- Issue of identifying overpotentials at high pH environments.

# ANODE (H<sub>2</sub>//O<sub>2</sub>/Air) continued..

## 2. Durability

- Role of oxygen crossover and ionomer/membrane stability at the anode interface.
- Other stability issues.

# Anode (liquid fuels)

1. Activity vs. selectivity – the best conditions for power density are not necessarily the best conditions for CO<sub>2</sub> selectivity
  - Effect of temperature
  - Effect of specific/non specific adsorption of cations in the context of selectivity
  - Role of contaminants
  - Unique electrostatics of the interface in the context of liquid fuels.
2. Role of specific adsorption of OH<sup>-</sup> in oxidation of liquid fuels
3. Reaction layer design - support material, interaction with ionomer – use of unsupported catalysts (prevalent for liquid fuel oxidation) can cause problems due to interfacial resistance between catalyst particles

# Cathode

## 1. Fundamental mechanistic issues

- Difference between acid and alkali – outer sphere / inner sphere
- Need for benchmarking – many papers compare new catalysts to Pt, but Pt may not be the best benchmark – Au and Pd can have higher activity. A proper benchmark catalyst both as single crystal surface as well as highly dispersed systems have yet to be identified. Here activity and long term stability are important considerations.
- Non-PGM – highly heterogeneous catalysts may have many kinds of active sites, and many processes may occur on the same active sites. Understanding ORR in the context of such complex reaction site environment is important., from a activity, selectivity and durability perspective.
- Separating effects of number of sites vs. turnover frequency is not generally done – also, site selectivity

# Cathode continued...

2. Hydrophobic/hydrophilic tailoring at the interface needed – different properties needed for H<sub>2</sub>/air vs. liquid fuel / air
3. CO<sub>2</sub> challenge:
  - Need systematic evaluation of CO<sub>2</sub> in terms of ionomer (exchange w.r.t OH<sup>-</sup> and lower conductivity) and Electrocatalysis (non availability of OH<sup>-</sup> species at the interface).
  - Effect of temperature – is there a sweet spot in terms of temperature above which CO<sub>2</sub> effects are mitigated (maybe around 80 C or higher?). 80C is in the context of current polymer chemistry.
  - Effect of potential on the possible interactions with the reaction site.

# Cathode continued....

## 4. Durability

- Active site, ionomer/catalyst (active site could catalyze ionomer destruction)
- Need to distinguish between degradation of different components (ionomer/catalyst/support)
- Mapping possible poisons both immediate as well as those which develop over time (aka from degradation processes in the ionomer/catalyst/support/stack components).
- Need for development of protocols and metrics for durability of ionomer in: (a) the membrane, (b) the catalyst layer, (c) the MEA
- Effect of peroxides on the stability of polymer electrolyte (ionomer and membrane) under cathode operating conditions (hydrogen crossover/potential).

# Interface

- A. O<sub>2</sub> permeability correlated with ionomer chemistry. How thick should coatings be?
- B. Hydration issues related to anode/cathode
- C. Ionomer aggregate structure – size and morphology of domains, and link with catalyst structure in the context of interfacial environment needs careful study.
- D. Specific studies on interfacial stability (ionomer degradation/delamination/morphology)
- E. Novel methods to investigation interfacial issues: structure, stability ect.
- F. New ideas on in situ polymerization of ionomer in the context of a catalyst layer.