Non-precious metal catalysts (NPMC) for proton exchange membrane fuel cells (PEMFC) are explored. Research into NPMCs is motivated by the growing need for cleaner, more efficient energy options. NPMCs are one option to make fuel cells more commercially viable. To this end, the present work studies and simulates the morphology and function of metal-nitrogen-carbon (MNC) oxygen reduction catalysts.

A porosity study finds that mesoporosity is critical to high performance of autogenic pressure metal-nitrogen-carbon (APMNC) oxygen reduction catalysts. Various carbon materials are used as precursors to synthesis APMNC catalysts. The catalysts and the associated porous carbon materials are characterized morphologically, chemically, and electrochemically. The results indicated that substrates adsorbing the most nitrogen and iron show the highest activity. Furthermore, a relationship is found between mesoporosity and nitrogen content indicating the importance of transport to active site creation.

A correlation is found between surface alkalinity and catalytic activity for APMNC catalysts. The basic site strength and quantity were calculated by two different methods, and it was shown that increased Brønsted-Lowry basicity correlates to more active catalysts. The relationship between alkalinity and catalytic activity could be the result of the impact of alkalinity on the electron density of the metal centers or basic sites could encourage active site formation.

It is found that the oxygen reduction reaction (ORR) proceeds both via a direct four-electron pathway to water at high potentials and an indirect peroxide pathway at low potentials on an APMNC catalyst. At higher potential, site availability inhibits peroxide generation causing the direct four-electron reduction pathway to dominate. Oxygen reduction begins to shift to the indirect peroxide pathway due to fast kinetics and higher site availability around 0.6 V vs RHE. The net peroxide generation remains relatively low over the entire range due to reduction of peroxide to water.
A PEMFC cathode model is developed for hydrophilic MNC catalysts. Water flooding was studied in terms of its impact on gas-phase transport and electrochemically accessible surface area (ECSA). Fuel cell data is modeled at a variety of pressures and catalyst layer thicknesses. A sensitivity study is performed on the controllable cathode parameters. Sensitivity analysis identified loading and density as critical parameters, and parametric studies indicated that decreased loading would lead to higher catalyst utilization. Also, density and loading of the catalyst layer are optimized for various fuel cell potential regions.

Persons with disabilities have the right to request and receive reasonable accommodation. Please call the Department of Chemical Engineering and Materials Science at 355-5135 at least one day prior to the seminar; requests received after this date will be met when possible.