

MAR13-2012-020104

Abstract for an Invited Paper  
for the MAR13 Meeting of  
the American Physical Society

**High-Performance Electrocatalysts for Oxygen Reduction Derived from Polyaniline, Iron, and Cobalt<sup>1</sup>**  
PIOTR ZELENAY, Los Alamos National Laboratory

With the growing awareness that the use of platinum needs to either be greatly reduced or completely eliminated from the polymer electrolyte fuel cell (PEFC), non-precious metal catalysts for oxygen reduction reaction (ORR) have received lots of attention in recent years as a possible replacement of Pt and its alloys at the fuel cell cathode. A successful cathode catalyst must combine high ORR activity with good long-term stability – a major challenge in the strongly acidic environment of the PEFC cathode. In response to the possibly greatest challenge of the PEFC technology, we have developed a family of non-precious metal ORR catalysts capable of minimizing the performance gap to platinum-based catalysts at a cost sustainable for high-power fuel cell applications, possibly including the automotive power plant. The approach utilizes polyaniline (PANI) as a precursor of a carbon-nitrogen template for high-temperature synthesis of catalysts in the presence of transition metals (Fe and/or Co). The most active materials in the group allow for the ORR to occur within ca. 60 mV of the potential delivered by a state-of-the-art carbon-supported Pt catalyst. A distinctive combination of (i) high ORR activity, (ii) unique performance stability for non-precious metal catalysts (more than 700 hours at a fuel cell voltage of 0.4 V), and (iii) excellent four-electron selectivity ( $\text{H}_2\text{O}_2$  yield less than 1.0%), make the leading catalyst in this group, PANI-FeCo(3:1), the best overall non-precious metal ORR catalyst studied to date. More recently, we have also focused on better understanding of the active ORR site via the use of advanced surface characterization techniques, such as nuclear resonance vibrational spectroscopy (NRVS), Monte Carlo pre-screening of possible active sites and more advanced DFT modeling of the most likely active-site structures. Combination of the experiment and theory is expected to aide in the rational design of the future ORR catalysts.

<sup>1</sup>Financial support from Los Alamos National Laboratory (LDRD Program) and US Department of Energy (Hydrogen and Fuel Cells Program) is gratefully acknowledged.