Sanjeev Mukerjee (A brief outline)

Dr. Sanjeev Mukerjee is a Professor in the Department of Chemistry and Chemical Biology (Northeastern University); where he has been since September of 1998. He also heads the newly created center for Renewable Energy Technology at Northeastern University and its subset the Laboratory for Electrochemical Advanced Power (LEAP). This center aims at enhancing education and research on all aspects of renewable energy and green chemistry with special emphasis on selective charge transfer at electrochemical and photo-electrochemical interfaces. His research on charge transfer dynamics at both two and three dimensional electrochemical interfaces encompasses materials development, *in situ* synchrotron spectroscopy and electro-analytical methods. In addition, new computational initiatives are in progress involving both molecular modeling and simulation of multiple electron scattering in the context of in situ synchrotron XANES method. Peer reviewed publication currently number 110, with an H-factor of 48. The current projects in the group include materials development for new electrocatalysts, polymer electrolyte membranes and high energy density (and capacity) cathode materials for aqueous and non-aqueous storage cells. Fundamental understanding of structure property relationships are in concert with applications.

Among the seminal contributions are, first demonstration of the power of true element specific in situ x-ray methods for understanding electrocatalysis and intercalation using synchrotron techniques of x-ray scattering and absorption. This was further enhanced by development of concerted simulation and subtractive methods, which further enabled study of surface adsorbed species with unprecedented insight. These in concert with materials development on supported noble and non noble metal nano-materials have shed important understanding of the nature of direct oxidation of complex fuels as well as oxygen reduction and evolution processes. New efforts are underway to create novel materials for photocatalytic oxygen evolution and free radical generation.

Translational activities in concert with fundamental research have lead to creation of two startup companies, Encite Corp, Burlington, MA and Protonex Corp., Westboro, MA. In addition partnership with De Nora, and BASF, Proton Onsite, Ford Motor Co., Advent North America and Automotive Fuel Cell Corporation (Canada) are ongoing for developing a number of fuel cell and electrolyzer technologies. Federal funding comes from the Army Research Office, Department of Energy, National Science Foundation, Air Force Office of Scientific Research and National Institute of Technology-Advanced Technology Program.

Novel Materials for Oxygen Reduction for Energy Storage and Conversion

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Oxygen reduction (ORR) and evolution reaction (OER) at an electrochemical interface has important connotations with several key technologies ranging from the use of oxygen depolarized cathodes in chlorine generation to fuel cells, electrolyzers, water treatment, hybrid batteries (including Li/Air) and even life support. In all the decades of research conducted in a wide range of pH (aqueous) and non aqueous electrolytes some very interesting threads have emerged pointing to revolutionary materials development. For example, recent advances in our understanding of alternative active sites for oxygen reduction has provided for the basis of its molecular design. This presentation will put these developments in the context of more than two decades of effort devoted to engendering such non noble metal electrocatalysts. In this presentation we will present our latest data on the most active analogs which comprise of a FeN_x coordinated active site in close concert with Fe nano-particles either present in some polymer composite or more ideally as edge defects close to the $Fe\text{-}N_x$ coordinated structure. We will show how these active sites evolve on carbon supports as graphene defect structures. Such active site determinations are made with the use of a special *in situ* synchrotron x-ray absorption method using the near edge spectra referred to as x-ray absorption near edge structure (XANES), in a subtractive mode wherein the signal contribution from the bulk is successfully subtracted from the effect of the surface adsorbed species. When combined with our ability to simulate the same signatures using models with specifically adsorbed moieties, a powerful tool emerges to study electrochemical interfaces under actual *in situ* and *operando* conditions. This technique, commonly called the 'Delta Mu ($\Delta\mu$) Technique' has been applied to a wide variety of transition metal surfaces and alloys[i,ii] including non-Pt based metal electrocatalysts with element specificity. EXAFS data taken concurrently provide information on the changes in short range atomic order around the absorber atom thereby providing structural information such as bond distances and coordination numbers (thereby information on average cluster size, homogeneity and surface segregation etc.).

In this presentation among other things we will provide a picture of the electrocatalytic pathways in aqueous (at both the extreme edges of the pH scale) and non-aqueous environments. In the latter, our prior efforts to understand the effect of electrolyte both in terms of solvent[iii] and choice of salt will be presented in terms of engendering inner our outer sphere charge transfer[iv] during ORR and OER reactions. The technological consequence of such materials in power generation, electrolysis and energy storage will be described.

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