

Adventures in Electrocatalysis for Clean Energy Conversion

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This talk will be devoted to electrocatalysis as a centerpiece of clean energy conversion by electrochemical means. Electrocatalysis has been the author's almost exclusive area of research since his master's and Ph.D. degrees studies in the Department, whose 70th anniversary we are celebrating these days.

We will begin with a brief look back at the early work on electrochemical adsorption by the radioactive labelling method conceived and successfully developed in the two no longer existing back wings of the Department's Radiochemistry Building and continued in the United States later. Radioactive labelling has proven to be the only truly quantitative method of measuring adsorption on solid electrodes, including adsorption of several key reaction intermediates relevant to the processes occurring in the direct-feed fuel cells.

Then, we will follow with an overview of the electrocatalysts developed for several key reactions occurring either at the fuel cell anode, e.g., methanol oxidation in the direct methanol fuel cell, or at the cathode such as oxygen reduction (ORR). In particular, we will concentrate on platinum group metal-free (PGM-free) ORR catalysts, including transition metal-nitrogen-carbon (M-N-C) materials. In addition to being a viable alternative to precious metals in fuel cells, M-N-C catalysts have been successfully implemented at Los Alamos for carbon dioxide reduction reaction (CO₂RR) to carbon monoxide. Finally, and time permitted, we will summarize the development of highly promising PGM-free catalysts for both hydrogen and oxygen evolution reactions designed for hydrogen generation via water splitting in anion exchange membrane water electrolyzers (AEMWEs).

Over the years, the catalyst development efforts at Los Alamos have been supported by advanced materials characterization techniques, as well as by the density functional theory (DFT) modeling and, more recently, adaptive learning (ML) methods. A few highlights from the latter efforts will be also included in this anniversary presentation.