

## Modeling Novel Catalysts for Fuel Cell Devices

Idupulapati N.B., and Mainardi D.S.

Institute for Micromanufacturing  
Louisiana Tech University  
Ruston, LA 71272

Recent advances in nano/bio technology are eliminating the past well known power output limitations that bio-fuel cells faced with respect to chemical fuel cells. Currently a biocatalytic fuel cell that uses bacterial Methanol Dehydrogenase (MDH) enzyme as the anodic catalyst and a chemical cathode, offers a potential attractive power source for consumer electronic devices producing a continuous power output of 100 mW. MDH is a quinoprotein that oxidizes methanol, and other primary alcohols to their corresponding aldehydes. The active site of MDH contains a  $\text{Ca}^{2+}$  ion, which is linked to pyrroloquinoline quinone (PQQ) and amino acids. The role of  $\text{Ca}^{2+}$  ion is not well understood. It has been suggested that apart from holding the PQQ molecule in place in the active site, the calcium ion might have an important role in the oxidation reaction mechanism. Moreover, the replacement of the  $\text{Ca}^{2+}$  in the MDH active site by other ion might modify the activation energy of the enzyme, facilitating the reaction by increasing the anodic current, which will contribute to enlarge the overall fuel cell power output.

Understanding the role of the ion in the active site of MDH, as well as the fuel oxidation mechanism will help to contribute to the design of novel catalysts for fuel cell applications. In this work  $\text{Ca}^{2+}$ -MDH and  $\text{Ba}^{2+}$ -MDH enzymes are being investigated to fully understand the methanol electro-oxidation reaction produced by these enzymes. Quantum mechanical Density Functional Theory (DFT) simulations are used to obtain geometry, energetic, electronic configurations, and information about the dissociation of methanol in the presence of the active site of these enzymes. Classical methods, such as Molecular Dynamics (MD) and Dynamic Monte Carlo (DMC) techniques are used to study the dynamics of the active site in the presence of the fuel, and to investigate the methanol electro-oxidation mechanism respectively through voltammetric scans.