Model development of enzymatic biofuel cells

Kim Pham and Tricia D. Shepherd
Dept. of Chemistry, St. Edward's University, Austin TX

Biofuel cells are batteries that employ biocatalysts. Enzymes are excellent fuel cell electron shuttles due to their high substrate specificity, being very selective in terms of what is oxidized or reduced. The ability of enzymes to utilize biologically-derived fuels, such as sugars, ascorbate, dopamine, and alcohols makes them viable as electric power sources in implantable devices in living organisms. Recently, scientists have been seeking to modify enzymes by adding graphitic attachments or various linker groups to increase their efficiency and longevity. Using molecular dynamic simulations, one can predict how an enzyme would interact with graphitic attachments in a system involving the transport of ions, gas and water - specifically biofuel cells. This project seeks to construct an atomistic model of the blue multi-copper oxidase laccase, run molecular dynamics simulations in water to calculate bond and angle parameters and the energy involved. Data from these simulations will be used to develop a coarse-grained model to study the transport of oxygen, ions and water at the interface between a fuel cell membrane, a graphitic surface, and the electrocatalytic enzyme laccase.