Computational studies of nanoparticles as fuel cell catalysts

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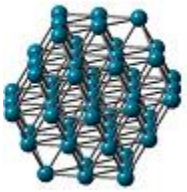

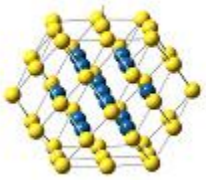

One of the obstacles in the fuel cell application is the kinetic limitation of oxygen reduction at the cathode at low temperatures. A major goal of this research project is to provide a fundamental understanding of the catalytic activity of transition metal nanomaterials on the oxygen reduction at an atomic and molecular level. For instance, between the two nanoparticles illustrated below, the pure Pt cluster (left) is not as active as the Pt/Au bimetallic cluster (right) in the oxygen reduction. Our research aims to provide understanding on the difference in their catalytic activity and to further predict even better catalytic candidates.

REU students will perform calculations using super computers to explore the size and structure effects on the oxygen reduction. Through the research activities, students will learn how to use the most common computational tools in both the academic and industrial worlds. The research project will also help students to understand better the abstract concepts that we often encounter in learning chemistry by “seeing how the atoms and molecules move”. Furthermore, students will gain experience on using supercomputers and state-of-the art software.