University at Buffalo
Department of Chemical and Biological Engineering
School of Engineering and Applied Sciences

October 24 | 11:00AM | 206 Furnas Hall

Guofeng Wang

Associate Professor

Department of Mechanical Engineering and Materials Science

University of Pittsburgh

Computational Design of Electrocatalysts for Proton Exchange Membrane Fuel Cells

Proton exchange membrane fuel cell (PEMFC) has attracted enormous attention as a viable, clean, and sustainable power generation technology alternative to widely employed fossil fuel-based technologies. Hydrogen oxidation reaction at the anode of a PEMFC is facile. In contrast, oxygen reduction reaction (ORR) at the cathode of PEMFC is sluggish due to a strong O-O bond in O_2 molecule and requires an efficient electrocatalyst for the effective reduction of O_2 to H_2O. Currently, platinum group metals (PGM) are found to be the best ORR electrocatalysts. The price of rare and expensive Pt-based electrocatalysts contributes significantly to the total cost of a fuel cell and hinders its mass application. Therefore, it is of great interest to investigate how to reduce and even eliminate PGM contents in the ORR electrocatalysts. In this seminar, I will present a computational study elaborating the ORR reaction mechanisms on Pt alloy catalysts and carbon-supported nitrogen-derived non-precious transition metal (TM-N/C, TM=Fe or Co) catalysts. Specifically, I will first discuss how the sub-surface transition metal could cause a shift in the d-electron band of the Pt alloy catalysts (such as, PtNi, PtCo and PtFe) and thus favorably modify the energetics of the ORR occurring on these Pt alloy catalysts. Moreover, I will examine the possible pathways of the ORR on the TM-N_4 clusters of the TM-N/C catalysts using the first-principles density functional theory calculation method. In particular, I will show that the ORR activity of the TM-N_4 clusters could be tuned by tailoring the energy levels of the non-bonding d-orbitals of the central TM atoms. Consequently, I demonstrate in this seminar that physics-based computational techniques are essential for accelerating, achieving, and amplifying research discoveries in the current forefronts of developing electrocatalysts for PEMFCs.

Wednesday Seminar Series