UC Irvine Samueli
Department of Chemical and Biomolecular Engineering

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Multiscale Modeling of Double Layer Effects in Electrocatalysis

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Abstract: Electrocatalytic reactions are central to advancing sustainable energy technologies and mitigating environmental impacts, particularly in renewable energy conversion and greenhouse gas reduction. Yet, the intricate structure of the electric double layer (EDL) poses significant challenges to understanding how electrolytes influence reaction mechanisms at electrified interfaces. In this talk, I will discuss a theoretical framework that integrates classical density functional theory (cDFT) for describing the diffuse layer, the Booth model for capturing the field-dependent dielectric behavior of the Stern layer, and Kohn-Sham density functional theory (KS-DFT) for resolving surface reactivity. This unified approach provides a self-consistent description of the interrelationships among electrode potential, surface charge density, interfacial electric field, Stern layer dielectric constant, and capacitance across diverse electrolyte conditions. By bridging atomic-scale surface properties with macroscopic experimental conditions, the multiscale framework offers mechanistic insights into ionic effects on electrocatalytic performance, enabling rational design and optimization of electrochemical systems.

Bio: Jianzhong Wu is a Professor in the Department of Chemical and Environmental Engineering at the University of California, Riverside, where he also holds collaborative appointments in Bioengineering, Materials Science and Engineering, and Mathematics. He earned his Ph.D. from the University of California, Berkeley, and his M.S. and B.S. degrees from Tsinghua University, Beijing. Professor Wu is an elected Fellow of both the American Physical Society (APS) and the American Institute for Medical and Biological Engineering (AIMBE), recognized for his contributions to classical density functional theory, molecular modeling, and interdisciplinary research in chemical engineering.

Hosted by: *Prof. Plamen Atanassov*