UCI Samueli School of Engineering

Department of Materials Science and Engineering UCI

UNIVERSITY OF CALIFORNIA, IRVINE

DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

IS PROUD TO HOST A SEMINAR BY

"MULTISCALE MODELING OF ELECTRIFIED INTERFACES IN BATTERIES"

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2:00 PM - 3:20 PM

McDonnell Douglas Engineering Auditorium

Abstract: Electrochemical interfaces are critical components that influence a wide array of technologies, including energy conversion and storage devices, air quality sensors, and water treatment systems. At electrified interfaces, charged species will re-distribute, forming an electric double layer (EDL). However, traditional continuum approaches underlying the century-old EDL framework often lack the atomistic details necessary to capture the complex interfacial phenomena observed in modern applications. Moreover, the classical Poisson–Boltzmann model—originally designed for fully solvated ions—proves increasingly inadequate for emerging electrolytes in advanced batteries, such as high concentration liquid electrolytes (HCE), localized high concentration liquid electrolytes (LHCE), and solid electrolytes (SE). This presentation aims to tackle the challenges by constructing predictive models of charged interfaces, specifically focusing on Li-metal/electrolyte interfaces in batteries. At these interfaces, two critical charge transfer reactions unfold: the desired ion transfer reaction of lithium during each charge/discharge cycle and a set of electron transfer reactions leading to the undesirable chemical decomposition of the electrolyte and the formation and growth of the solid electrolyte interphase (SEI). To address these challenges, we start with density functional theory (DFT)-informed continuum models to discuss the electric potential alignments in both full cell and half-cell configurations, encompassing both solid and liquid electrolytes. After determining the surface charge state at Li-plating, an interactive Molecular Dynamics - DFT - data statistics model is developed to analyze the reduction reactions of multicomponent electrolytes within the EDL. The interplay among cations, anions, and various solvent species with a charged surface at different temperatures collectively influences the EDL structure and, consequently, the composition of the SEI. These predictions are supported by experimental measurements. They not only provide valuable insights but also offer guidance and a toolset for the direct design of interfaces in batteries.

Bio: Dr. Yue Qi is the Joan Wernig Sorensen Professor of Engineering at Brown University and serves as the Deputy Director of the Initiative for Sustainable Energy (ISE). She earned her B.S. in Materials Science and Engineering and Computer Science from Tsinghua University, followed by her Ph.D. from Caltech. For 12 years, she worked at General Motors R&D, developing multi-scale models to solve engineering challenges related to lightweight materials, fuel cells, and batteries. In 2013, she transitioned to academia, initially joining Michigan State University before moving to Brown University. Dr. Qi's research focuses on multi-scale and multi-physics simulations, which are key to designing materials and interfaces critical to energy-efficient technologies. She has been recognized with several research awards, including the Feynman Prize in Nanotechnology and the Brimacombe Medal from the Minerals, Metals & Materials Society (TMS).