Special Guest Lectures

Chemistry at Interfaces: From the Air-Water to the Electrode-Electrolyte Interface

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Abstract:

Chemical processes at interfaces are of importance in a wide range of systems, ranging from biological membranes, to industrial applications, to atmospheric and even geological systems. My research focuses on two important interfaces: the air-water interface and the electrode-electrolyte interface in Li-ion batteries. The acidic nature of the air-water interface is a topic of intense debate. Spectroscopic evidence points to the presence of protons at the interface while electrophoresis experiments suggest the presence of the hydroxide anion. Molecular Dynamics (MD) simulations are particularly challenging because the proton and the hydroxide ion can hop between water molecules necessitating a model that allows for chemical reactivity. I will discuss the development of a reactive model for the proton and hydroxide ion and the interesting insight provided from MD simulations of the aqueous solution-air interface utilizing this model. The complex solid electrolyte interface (SEI) in rechargeable Li ion batteries, which forms as a result of electrolytic reactions, acts as a passivating layer to protect the electrode and greatly impacts battery performance. Atomistic level simulations can provide critical understanding of the mechanism of Li+ ion transport through the SEI. While ideally one would prefer to use ab initio MD simulations, the long time and length scales associated with this system make this computationally intractable. The force-matching method allows one to bridge the gap between computationally expensive ab initio methods and simple force-fields. I will discuss the algorithm to develop robust models for the electrode-electrolyte and the results on the structure of the electrolyte at the electrode surface as a function of applied voltage.

Speaker's Bio:

Revati Kumar did her PhD in theoretical chemistry at the University of Wisconsin-Madison. She is current a postdoctoral researcher in Prof. Gregory Voth's group at the University of Chicago. Her research focuses on modeling chemical systems and lies at the intersection of Statistical Mechanics and Quantum Chemistry (electronic structure).

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