Lithium Ion Batteries are currently the electrochemical devices used to enable electric vehicles. Many battery components are only metastable at the high voltage operating conditions, leading to degradation of performance over time, and even failure and safety concerns. It can be argued that every battery material research experimental paper is also about the degradation of that material as cycling proceeds. In contrast, traditional atomic lengthscale modeling of battery materials and interfaces focused on time-in dependent, thermodynamic analysis.

In this theory/modeling talk, we will present electronic structure studies of chemical and/or electrochemical reactions responsible for the degradation but also the stabilization and evolution of battery interfaces. We will focus on reaction barriers which can be extrapolated to reaction lifetimes. Voltage dependences will be emphasized, and addressed in a unified framework that applies to both batteries and other electrochemical devices, such as fuel cells and supercapacitors. Battery interfaces associated with solid- and liquid-state electrolytes will be compared. These discussions will be preceded by a brief overview of battery science and technology. and another by the dilution effects due to entropy. The canonical PS-PEO system is expected to be in the solvation regime.

Biography

Kevin Leung received B.A. degrees in Physics and Chemistry from the University of Rochester in 1989 and Ph.D in Physical Chemistry from the University of California at Berkeley at 1994. He was a postdoctoral fellow at the University of Southern California in 1995 and at Berkeley in 1996-1997. He joined Sandia as a limited term staff in 1997 and became a Senior Member of the Technical Staff in 1999 and a Principal Member of the Technical Staff in 2006. He has worked in diverse areas including solid materials, liquids, and liquid-solid interfaces.