Using computational materials physics to understand and improve battery performance

Michelle Johannes

Section Head, Center for Computational Materials Science
Naval Research Laboratory

Although batteries are generally considered electrochemical systems, a surprising amount of their performance stems from the physics of the materials that make up their basic components: anode, cathode, and electrolyte. Ionic conduction, electronic conductivity, chemical stability, and voltage can all be traced back to intrinsic material properties which are governed by fundamental physics. In this talk, I will discuss how computational simulations can be used to gauge the utility of oxide and phosphate materials for use in Li-ion battery materials. I will specifically discuss how seemingly small details of the electronic structure of electrode materials can make or break battery performance. I will further discuss some of the safety concerns that are currently driving battery research and development and how computational screening can determine in advance how stable a material will be during charging. Finally, I will discuss the use of nanoscale materials and how they can be stabilized against degradation by judicious oxide coating.