MSE SPECIAL SEMINAR

MATERIALS SCIENCE & ENGINEERING | SPRING 2018

THURSDAY, APRIL 5, 2018 | 243 WILCOX HALL | 3:30 PM

The Materials Physics of Intercalation-Driven Structural Transformations in Layered Battery Materials

One of the factors limiting the performance of Li- and Na-ion batteries is the complex structural transformations that occur upon intercalation. This includes crystallographic transformations involving changes in the stacking of layers, as well as phase transitions associated with collective Jahn-Teller distortions. Many questions remain about how these transformations affect battery performance and contribute to the fracture and mechanical damage that limits cycle life. Here we present new models to capture the coupling between intercalation chemistry and mechanics arising from such structural transformations. This includes first-principles simulations and mesoscale models to elucidate the thermodynamics and kinetics of stacking-sequence changes, as well as anharmonic vibrational models to describe the transition from a static to dynamic Jahn-Teller distortion. Key results include understanding why different intercalants yield different stacking-sequence changes, and how stacking-sequence changes can result in irreversible changes to microstructure. Regarding Jahn-Teller distortions, numerical simulations reveal how the interplay between the shape of the Jahn-Teller energy landscape and rigidity of the crystal impact the local structure and thermodynamic properties of dynamically distorted phases.

Maxwell Radin

Postdoctoral Scholar
Materials Department
University of California, Santa Barbara

Maxwell D. Radin received his B.S. in Physics from the University of California, Irvine, and Ph.D. in Physics from the University of Michigan. His Ph.D. research, advised by Donald J. Siegel, focused on modeling point defects and charge transport in materials for Li/O2 batteries, and was recognized with the ProQuest Distinguished Dissertation Award. As postdoctoral scholar at the University of California, Santa Barbara (advised by Anton Van der Ven), his current research focuses on modeling from first-principles the coupling between intercalation chemistry and mechanics in battery materials.

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