FAKULTÄT FÜR CHEMIE

universität wien

Einladung zum Vortrag von

Prof. Dmitry Bedrov

University of Utah, Salt Lake City

„Multiscale modeling of nanostructured electrodes and interfaces in Li-ion batteries”

In this talk I will discuss interdisciplinary efforts on multiscale modeling of electrochemical devices undertaken at the Alliance for Computationally-guided Design of Energy Efficient Electronic Materials (CDE3M). Specifically I will focus on our recent results in modeling of components of Li-ion batteries, including solid electrolyte interphase (SEI), SEI/electrolyte interfaces, and nanostructured Si anodes. The coupling of electrochemical and mechanical processes inside electrodes and at electrode/SEI interfaces is one of the key challenges that has to be addressed in order to provide efficient materials-by-design of novel batteries. Most of the current modeling tools only consider a continuum level modeling and do not couple the atomic and molecular scale processes explicitly. Instead, the effects of these key phenomena are introduced by empirically adjusting constitutive model parameters. We have focused on developing a set of multiscale modeling tools that allows us to couple the atomic, molecular and nanoscale electrochemical and mechanical processes to continuum level modeling.

Montag, 17. Juli 2017, 10:00 Uhr

Seminarraum

Währingerstraße 17, 1090 Wien

Christian Schröder

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Bernhard Keppler
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