

Carnegie Mellon University

Materials Science & Engineering

presents

Simulations of Energy Materials

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Electrochemical systems play an important role in environmentally sustainable energy conversion and storage. Electrochemical processes involve transport through multiple phases (electrolyte and electrodes) and reactions at electrode surfaces having complex geometries. Therefore, simulation-based studies of reaction and diffusion processes using a realistic microstructure help us elucidate the microstructural effects on the performance of electrochemical systems. In this presentation, I will first provide an overview of how simulations are used in advancing our understanding of materials for energy applications. I will then focus on simulations of battery cathodes during charge-discharge cycles. The numerical approaches such as phase field modeling and the smoothed boundary method used in the simulations are also described. The interplay of electrochemistry, thermodynamics, and kinetics are illustrated through the simulation results, and their implications to experimental and materials design will be discussed.

Katsuyo Thornton is an associate professor of materials science and engineering at the University of Michigan, Ann Arbor. Her research focus is on computational studies of the evolution of microstructures and their effects in a wide range of materials, including metals, semiconductors, oxides, and biomaterials. She received her Ph.D. from the Department of Astronomy and Astrophysics at the University of Chicago in 1997. She was a Postdoctoral Fellow at Northwestern University and a Visiting Lecturer and Scientist at MIT, both in Materials Science and Engineering, followed by three years as a Research Assistant Professor in Materials Science and Engineering at Northwestern University. She has served in a leadership role as the inaugural Chair of the Integrated Computational Materials Engineering (ICME) Committee within TMS and as a co-organizer of the 2013 ICME Congress. She established the Summer School for Integrated Computational Materials Education in 2011, and she continues to hold the event annually. These activities are being recognized by TMS through the 2015 TMS Materials Processing & Manufacturing Division Distinguished Service Award. She is also the recipient of several prestigious awards, including the TMS Early Career Faculty Fellow Award, the NSF Faculty Early Career Development (CAREER) Award, and the Carl Sagan Excellence in Teaching Award.

Doherty Hall 2210, 11:30AM
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