Condensed Matter / Biophysics Seminar

Simulations of Morphological Evolution in Energy Models

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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 and anodes 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.

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