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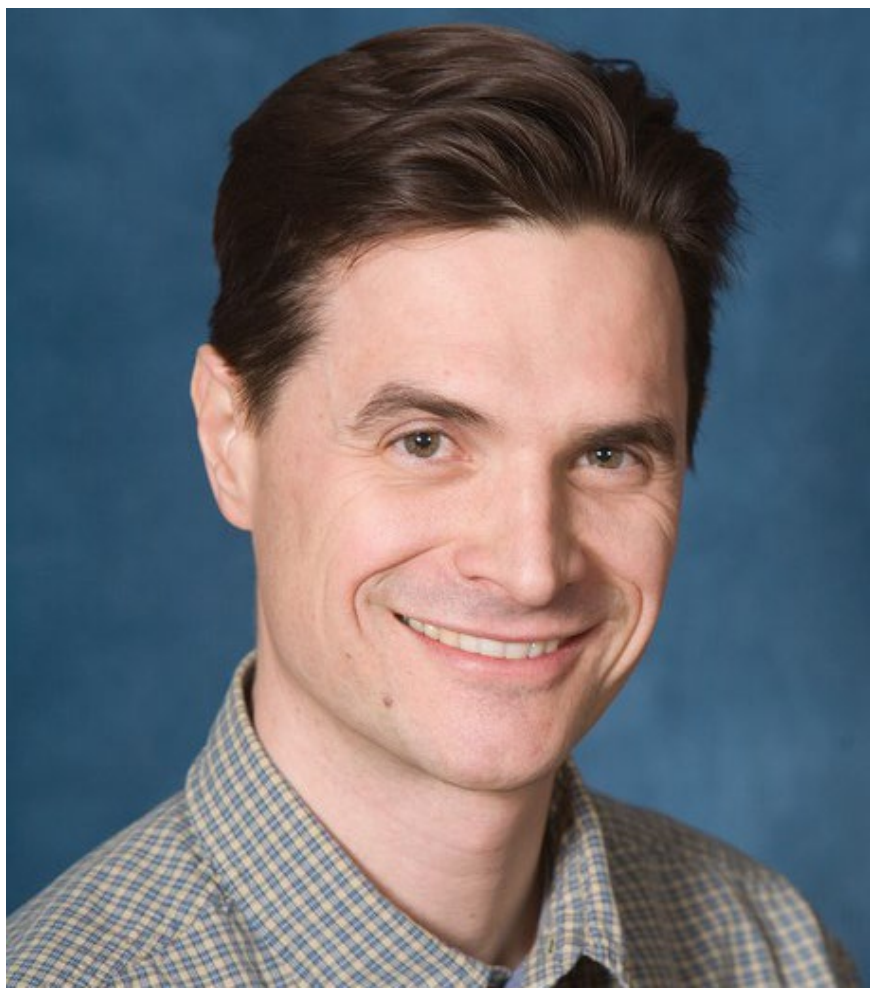
Chemistry & Biochemistry

PHYSICAL CHEMISTRY SEMINAR



Prof. Anton Van der Ven

College of Engineering, Materials Department
University of California, Santa Barbara

Monday, February 13, 2023

4:00 PM | YH 4222

Mani L. Bhaumik Collaboratory -

Dongwon Yoo Seminar & Conference Hall

From Electronic Structure to Battery Thermodynamics and Kinetics

Abstract: Most electrochemical processes can be modeled with powerful phenomenological theories that describe ion transport, interface reactions and mechanical responses. Phenomenological descriptions, however, rely on materials specific coefficients and free energies, which are quantities that are often difficult to measure in isolation. An alternative to an experimental approach is to predict these quantities from first principles. Since electrochemical processes are thermally activated, temperature and entropy play an important role. The prediction of materials properties, therefore, requires a statistical mechanics approach. In this talk I will describe a generalized framework with which to connect the electronic structure of crystalline solids to their equilibrium and kinetic properties at the macroscopic scale. I will illustrate how the application of first-principles statistical mechanics can generate crucial ingredients for phenomenological models of electrochemical processes, including composition dependent free energies and open circuit voltage profiles, ionic transport coefficients and chemo-mechanical response functions. The capability to predict thermodynamic and kinetic properties of electrode materials is allowing us to explore and design new battery chemistries and concepts. Electrode materials for Li, Na and Mg ion batteries undergo a series of phase transformations as a result of large changes in concentration during each charge and discharge cycle. While the mechanisms of these phase transformations remain poorly characterized, they can to an extent be understood with first-principles multi-scale approaches.

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