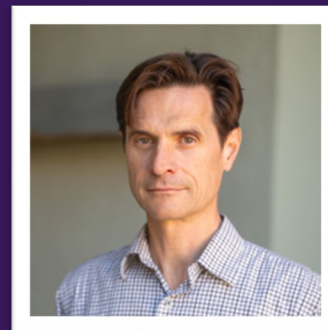


THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT
FALL COLLOQUIUM SERIES PRESENTS:

Professor Anton Van Der Ven

Professor of Materials Department

University of California – Santa Barbara



Ion transport and phase transformation mechanisms in battery materials

Batteries are extraordinary devices when viewed from the vantage point of a materials scientist. They rely on the shuttling of mobile cations such as Li or Na between metallic electrodes that are separated by an electronically insulating electrolyte. This induces large swings in the cation concentration of the electrode materials and often results in a variety of structural and ordering phase transformations. Viable electrode materials tend to have complex crystal structures, which can lead to unique ionic transport mechanisms. Cathode materials are transition metal oxides and often exhibit peculiar electronic and magnetic properties that vary during the course of charging and discharging the battery. Furthermore, large volume and shape changes of the electrode materials during each charge and discharge cycle can cause complex chemo-mechanical phenomena that need to be understood and controlled in order to extend the lifetime of battery materials. Increasingly, modern computational approaches are being used to predict and understand the intriguing electrochemical properties of battery materials. In this talk I will describe first-principles statistical mechanics methods that are able to predict the thermodynamic and kinetic properties of electrode materials for Li-ion and Na-ion batteries. These methods have shed light on the link between the electronic structure of electrode materials and their electrochemical properties and have revealed a rich variety of ionic diffusion mechanisms in the solid state. I will focus in particular on intercalation compounds, commonly used as cathodes, and lithium alloys, which are currently of great interest due to their ability to foster uniform plating and stripping of lithium in all-solid-state batteries.

Anton Van der Ven is Professor in Materials at UC Santa Barbara. His research focuses on the development and application of first-principles statistical mechanics methods for the prediction of the thermodynamic and kinetic properties of metal alloys, ceramics and semiconductor compounds. He joined UC Santa Barbara in 2013 after starting his academic career at the University of Michigan. He received his PhD from the Massachusetts Institute of Technology in 2000 and continued on as a postdoctoral researcher until 2004. Van der Ven is the recipient of the TMS Hume-Rothery award and several teaching awards.

Tuesday, Nov. 3 • 4 pm CT • Tech L211

In person only; no Zoom

Questions? Contact allison.macknick@northwestern.edu