Nebraska Engineering

**FACULTY CANDIDATE SEMINAR**

University of Nebraska-Lincoln
Department of Chemical and Biomolecular Engineering

# Understanding Defect Behavior in Advanced Materials Through Ab Initio Based Multiscale Modeling


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2:30 p.m. – 4:00 p.m.
Othmer Hall, Room 205
**Refreshments provided*


## Abstract

Atomic-scale defects are part and parcel of real solids and often determine macroscale behavior of materials. Quantum-mechanical based computational methods can provide microscopic information about the underlying mechanisms of defect behavior in advanced materials, however it is often unclear how to properly upscale these details through the mesoscale to the macroscale. Using a multi-scale computational approach involving density functional-theory (DFT) calculations, cluster expansion, Monte Carlo simulations and continuum elasticity analyses I show how one can establish relationships between thermodynamics, defect clustering and oxygen-ion conductivity in solid solutions of fluorite-based oxide ceramics. The results will be discussed in the context of solid electrolyte and nuclear energy applications. In the second part I will show how macroscopic electrical conductivity based on electron small-polaron hopping can be computed from microscopic first principles simulations, for a number of redox-active iron-bearing oxides. Specifically, I will discuss the speciation of aqueous Fe(II) at oxide surfaces, and mechanisms of bulk and interfacial Fe(II)-Fe(III) electron transfer based on the DFT calculations aided by ab initio molecular dynamics simulations. Finally, I will highlight the interplay between various structural defects and charge/ion transport properties relevant for corrosion/oxidation of Nibased superalloys, mechanical properties of ceramic oxides and a number of solid-state electrochemical applications.