



University at Buffalo

Department of Materials  
Design and Innovation

School of Engineering and Applied Sciences  
College of Arts and Sciences

## CAS / SEAS SEMINAR

### **Ferroionics at the Nanoscale: when Ferroelectricity meets Electrochemistry A Study by Mesoscale Phase-field Modeling**

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**Abstract:** Functional materials such as ferroelectric oxides underpin a vast spectrum of modern technological applications such as nonvolatile memories, piezoelectric actuators/sensors, and dielectric/ferroelectric capacitors. A fundamental understanding of the microstructural evolutions in nanoscale functional oxide, such as ionic motion, ferroelectric domain evolution and phase transition, and their couplings with thermal, electrical, mechanical and chemical excitations are fundamental to the realization of many of its application. In this presentation, Dr. Cao will demonstrate a mesoscale computational approach to this problem, based on the phase-field modeling of ferroelectric microstructure evolution and defect chemistry/kinetics for ionic and electronic transport. The first part of the presentation concerns the roles of surface and electrochemical phenomena in the stability and switching dynamics in lead zirconate titanate thin film, ranging from surface chemical effect, to flexoelectric effect (inhomogeneous strain gradient), and to bulk oxygen vacancy dynamics. The second part of the presentation will discuss the ionic transport and resistance degradation phenomena in barium titanate based ferroelectric capacitor. Dr. Cao will explore the interactions among ferroelectric domain state, oxygen vacancy distribution and diffusion, and leakage current evolution. Finally, the implication of these examples, as well as the potential application of the established mesoscale model will be discussed to provide insights for the future design and optimization of energy related materials.

**BiO:** Ye Cao obtained his B.Sc. and M. Sc. from Shanghai Jiao Tong University in China, and his Ph.D. in Materials Science and Engineering from the Pennsylvania State University in 2014 under the supervision of Prof. Long-Qing Chen. He is now working with Dr. Sergei V. Kalinin as a Postdoc Research Associate at Oak Ridge National Laboratory. His research interests are mesoscale phase-field simulations on the microstructural evolutions and applications in functional oxides, such as ionic/electronic transport and resistance degradation in ferroelectric capacitors, domain switching and phase transition in ferroelectric thin film, and electric, elastic and chemical coupling in nanoscale functional oxides.

**Date:** Monday, April 10  
**Location:** 280 Park Hall, North Campus

**Time:** 1:30 pm