MATERIALS SCIENCE & ENGINEERING SEMINAR, NH 203
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Learning the mesoscopic and atomic physics of ferroelectrics: imaging and big data

Abstract:
Ferroelectricity on the nanoscale has remained a subject of much fascination in condensed matter physics for the last several decades. It is well-recognized that stability of the ferroelectric state necessitates effective polarization screening, and hence screening mechanism and screening charge dynamics become strongly coupled to ferroelectric phase stability and domain behavior. Similarly, atomic scale defects can strongly affect polarization stability and affect wall pinning and nucleation and give rise to relaxor states. In this presentation, I will illustrate several recent results on ferroelectric and ferroic – chemical coupling on mesoscopic and atomic scales. In the nanoscale systems, the ferroelectric state is fundamentally inseparable from electrochemical state of the surface, leading to emergence of coupled electrochemical-ferroelectric states. I will present the results of experimental and theoretical work exploring the basic mechanisms of emergence of these coupled states including the basic theory and phase-field formulation for domain evolution. I further discuss the thermodynamics and thickness evolution of this state using analytical theory and phase-field modelling. These considerations further stimulate the development of the novel SPM modalities addressing time-dependent dynamics and chemical changes during SPM imaging. I will further delineate the applications of in-situ SPM – time of flight secondary ion mass spectrometry (ToF SIMS) to map the changes in surface chemistry during tribological and local electrochemical experiments, including ferroelectric polarization switching and pressure-induced resistance changes in oxides. On the atomic scales, significant inroads in local ferroelectric behaviors can be obtained from atomically-resolved studies of ferroelectric materials that allow direct visualization of materials structures and order parameter fields. These approaches further necessitate analysis and data mining of large volumes of information, and first examples of deep learning analysis on STEM data to infer local materials behavior and kinetics of point-defect reactions will be illustrated.

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About the Speaker:
Sergei V. Kalinin is the director of the ORNL Institute for Functional Imaging of Materials and distinguished research staff member at the Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (at ORNL since 2002). He also holds a Joint Associate Professor position at the Department of Materials Science and Engineering at the University of Tennessee-Knoxville, and an Adjunct Faculty position at Pennsylvania State University. His research interests include application of big data, deep data, and smart data approaches in atomically resolved and mesoscopic imaging to guide the development of advanced materials for energy and information technologies, as well as electromechanical, electrical, and transport phenomena and matter patterning on the nanoscale via scanning probe and electron microscopy.

He received his Ph.D. from the University of Pennsylvania in 2002, followed by a Wigner fellowship at ORNL (2002-2004). He is a fellow of APS, IoP, IEEE, MRS, Foresight Institute, and AVS; a recipient of the Blavatnik Award in Physics (2018), RMS medal for Scanning Probe Microscopy (2015); Presidential Early Career Award for Scientists and Engineers (PECASE) (2009); IEEE-UFFC Ferroelectrics Young Investigator Award (2010); Burton medal of Microscopy Society of America (2010); ISIF Young Investigator Award (2009); American Vacuum Society Peter Mark Memorial Award (2008); 3 R&D100 Awards (2008, 2010, and 2016); Ross Coffin Award (2003); Robert L. Coble Award of American Ceramics Society (2009); and a number of other distinctions. He has published more than 600 peer-reviewed journal papers, edited 3 books, and holds more than 18 patents. He has organized numerous symposia (including symposia on Scanning Probe Microscopy on Materials Research Society Fall meeting in 2004, 2007, and 2009) and workshops (including International workshop series on PFM and Nanoferroelectrics), and acted as consultant for companies such as Intel and several scanning probe microscopy manufacturers. He is also a member of editorial boards for several international journals, including \textit{Journal of Applied Physics/ Applied Physics Letters}, and recently established Nature Partner Journal \textit{Computational Materials}.

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