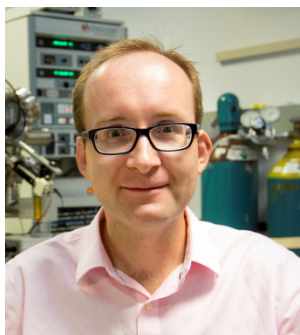


**Big, Deep, and Smart Data in Energy Materials Research:  
Atomic View on Materials Functionalities****Sergei V. Kalinin**

Oak Ridge National Laboratory

**September 22, 2015 (Tuesday) | 1.00pm**  
**D172, Building 241, Argonne National Lab**

**ABSTRACT** Structural and electronic properties of oxide surfaces control their physical functionalities and electrocatalytic activity, and are currently of interest for energy generation and storage applications. In this presentation, I will discuss several examples of high-resolution studies of the electronic and electrochemical properties of oxide surfaces enabled by multidimensional scanning probe microscopies. On the mesoscopic scale, combination of strain- and current sensitive scanning probe microscopies allows to build nanometer-scale maps of local reversible and irreversible electrochemical activities. The use of multivariate statistical methods allows separating the complex multidimensional data sets into statistically significant components which in certain cases can be mapped onto individual physical mechanisms. I will further discuss the use of *in-situ* Pulsed Laser Deposition growth combined with atomic resolution Scanning Tunneling Microscopy and Spectroscopy to explore surface structures and electrochemical reactivity of oxides on the atomic scale. For  $\text{SrRuO}_3$ , we directly observe multiple surface reconstructions and link these to the metal-insulator transitions as ascertained by UPS methods. On  $\text{La}_x\text{Ca}_{1-x}\text{MnO}_3$ , we demonstrate strong termination dependence of electronic properties and presence of disordered oxygen ad-atoms. The growth dynamics and surface terminations of these films are discussed, along with single-atom electrochemistry experiments performed by STM. Finally, I explore the opportunities for atomically-resolved imaging and property data mining of functional oxides extending beyond classical order parameter descriptions, and giving rise to the deep data analysis in materials research.



*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, as well as a theme leader for Electronic and Ionic Functionality on the Nanoscale (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 coupling between electromechanical, electrical, and transport phenomena on the nanoscale.*