Machine Learning in Microscopy: from Materials Design to Atom-by-Atom Assembly

Sergei V. Kalinin

The Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831

Machine learning and artificial intelligence (ML/AI) are rapidly becoming an indispensable part of physics research, with domain applications ranging from theory and materials prediction to high-throughput data analysis. In parallel, the recent successes in applying ML/AI methods for autonomous systems from robotics through self-driving cars to organic and inorganic synthesis are generating enthusiasm for the potential of these techniques to enable automated and autonomous experiment (AE) in imaging. In this presentation, I will discuss challenges and opportunities of AE in STEM, ranging from feature discovery to learning physics and controlled intervention. The special emphasis is made on the rotationally invariant variational autoencoders that allow to disentangle rotational degrees of freedom from other latent variables in imaging and spectral data. The analysis of the latent space of autoencoders further allows establishing physically relevant transformation mechanisms. Extension of encoder approach towards establishing structure-property relationships will be illustrated on the example of plasmonic structures. I further discuss the strategies based on Gaussian Processes for automated experiment, and demonstrate some initial results for AE in STEM and potential applications for electron beam manipulation of matter on mesoscopic and atomic level towards fabrications of plasmonic structures with desired properties and single-atom devices.

This research is supported by the by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division and the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, BES DOE.

About Sergei V. Kalinin:

Sergei Kalinin is a corporate fellow and a group leader at the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory. He received his MS degree from Moscow State University in 1998 and Ph.D. from the University of Pennsylvania (with Dawn Bonnell) in 2002. His research presently focuses on the applications of big data and artificial intelligence methods in atomically resolved imaging by scanning transmission electron microscopy and scanning probes for applications including physics discovery and atomic fabrication, as well as mesoscopic studies of electrochemical, ferroelectric, and transport phenomena via scanning probe microscopy.

Sergei has co-authored >650 publications, with a total citation of >38,000 and an h-index of >95. He is a member of Academia Europea and a fellow of MSA, MRS, APS, IoP, IEEE, Foresight Institute, and AVS; a recipient of the Blavatnik Award for Physical Sciences (2018), RMS medal for Scanning Probe Microscopy (2015), Presidential Early Career Award for Scientists and Engineers (PECASE) (2009); Burton medal of Microscopy Society of America (2010); 4 R&D100 Awards (2008, 2010, 2016, and 2018); and a number of other distinctions.