UCLA College | Physical Sciences Chemistry & Biochemistry

PHYSICAL CHEMISTRY SEMINAR

Sergei V. Kalinin, Ph.D.
Distinguished Research Staff Member,
The Center for Nanophase Materials Sciences
Oak Ridge National Laboratory

Monday, June 1, 2020
4:00 PM
via Zoom

“Machine Learning Beyond Correlative Models: Bayesianity, Parsimony, Causality, and Automated Experiment”

Machine learning has emerged as a powerful tool for the analysis of mesoscopic and atomically resolved images and spectroscopy in electron and scanning probe microscopy. The applications ranging from feature extraction to information compression and elucidation of relevant order parameters to inversion of imaging data to reconstruct structural models have been demonstrated. However, the fundamental limitation of the vast majority of machine learning methods is their correlative nature, leading to extreme susceptibility to confounding factors and observational biases. While in classical statistical methods the methodology to address phenomena such as Simpson paradox are established, the complex and often non-transparent nature of modern DL tools renders them extremely prone to misinterpretation. We argue that correlative machine learning provides a reliable and powerful tool in cases when the causal links are well established, and discuss several examples of atom finding in SPM and STEM and analysis of 4D STEM data when this condition is satisfied. Notably, ML applications in theory generally fall under this category sine the causal mechanisms are postulated. Alternatively, ML methods work well when the confounding factors are effectively frozen via the narrowness of experimental conditions or experimental system. However, both these conditions are violated for experimental studies, when causal relationships are known only partially (and are in fact often the target of study) and confounding and latent factors (composition uncertainty, microscope tuning, contaminations) are abundant.

In this presentation, I will discuss the several examples of extending machine learning methods towards the analysis of causative physical mechanisms. One such approach is based on the Bayesian methods that allow to take into consideration the prior knowledge the system and evaluate the changes in understanding of the behaviors given new experimental data. The second pathway explores the parsimony of physical laws and aims to extract these from the set of real-world observations. Finally, the Bayesian networks can be used to explore the causative relationships in the multimodal data sets. These concepts will be illustrated using several examples of causal machine learning, including analysis of phase transitions on a single atom level in 2D materials and interplay between physical and chemical effects in the ferroelectric perovskites. Ultimately, we seek to answer the questions such as whether electronic instability due to the average Fermi level guides the development of the local atomic structure, or frozen atomic disorder drives the emergence of the local structural distortions, whether the nucleation spot of phase transition can be predicted based on observations before the transition, and what is the driving forces controlling the emergence of unique functionalities of morphotropic materials and ferroelectric relaxors. The unique aspect of Bayesian methods is their potential to quantify uncertainty, and harnessing this for automated experimentation is discussed on example of ferroelectric domain patterning and atomic fabrication via electron beams.

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.

Please contact marla@chem.ucla.edu for additional information.