Automated Experiments, Machine Learning and Reinforcement Learning for tuning and control applications in microscopy*

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Abstract

Machine learning has offered a new tool that can be used towards tuning and control of material properties, whether it be during the design, synthesis or characterization stages of the process. In this talk, we will discuss our work on using machine learning and reinforcement learning for all three stages.

First, we will explore the use of reinforcement learning agents for the tuning of ferroelectric material properties via appropriate positioning of point defects in a ferroelectric lattice, through simulations. By engineering the reward function, it becomes possible to tune the properties towards such novel features as maximizing curl in the order parameter field, or minimizing piezoelectric response in certain orientations.

Next, we will show that machine learning, and computer vision approaches can be used as a tool during synthesis and characterization, to tailor applied excitations to elicit a desired response. It is shown, for example, that moving ferroelectric domain walls to regions of high frustration can drive the state to one in which the wall is far more labile, thereby increasing the electromechanical response locally.

Finally, we discuss how Bayesian optimization methods can be best utilized to improve characterization via efficient, adaptive sampling in the presence of prior knowledge, typically from high-resolution imaging conducted before the (longer-duration) spectroscopy. This combination can lead to adaptive control over instrument parameters that maximizes physics knowledge extraction, as opposed to simply minimizing uncertainty as is the usual metric for most problems outside of basic science. This work was performed at and supported by the Center for Nanophase Materials Sciences, a US DOE Office of Science User Facility.

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