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Meeting-report

Human-in-the-Loop Automated Experiment Simulated with Scanning Tunneling Microscopy

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Recently, scientific discoveries have been accelerated by using machine learning to analyze the data post-experiment. However, it's still a rare case to use machine learning to help data acquisition during the experiment. Such attempt has been proven successful in the form of deep kernel learning (DKL) for piezoelectric force microscopy [1] and combinatorial library exploration [2] with scanning probe microscopy based on human in the loop automated experiment (hAE). It not only offers high-throughput characterization of materials, but also enables studying systems with giant amounts of data that human researchers cannot handle. In a typical hAE workflow, human operators provide the reward function to define the goal of the experiment and experiment policy to guide the behavior of the machines. Then the machine learning will learn the correlation within the acquired data and determine the next location for the next measurement based on reward function and policy. In this talk, I will present the hAE simulation based on complete STM data pre-acquired on various quantum materials, showing the possibility of accelerating physics research with hAE.

First, I will show variational autoencoder (VAE) analysis and simulation of DKL hAE on complete STM grid data taken on topological Kondo insulator SmB6 [3, 4]. In SmB6, the formation of Kondo holes around Sm-site defects creates charge puddles around them, which leads to change in the rectification and zero-bias point in the I-V curve around them. Here I show that the DKL can predict the charge puddles formed around Kondo holes and its model uncertainty from the topography image after only 200 local conductance measurements (iterations). Then I will show another VAE + DKL simulation on the high-Tc superconductor BSCCO [5]. In BSCCO, the local doping level determines the local superconducting gap size that can be measured by the local differential conductance spectroscopy. This variation of superconducting gap size further decides the variation of superconducting transition temperature in the material. In this example, the DKL can predict the local gap size based on analysis of the local doping level in the topography image. These two examples indicate that hAE with STM can learn the relation between the structural features in the topography image and physical properties revealed in the spectra without the necessity of taking the full grid-measurement. Therefore, hAE has the potential to greatly accelerate physics research with STM.

This VAE + DKL workflow is universal as it does not require any special knowledge about STM. Therefore, it can be applied to automate any SPM and electron microscopy (EM) techniques, including force-distance measurements in AFM, hysteresis loop measurements in PFM, I-V measurements in cAFM and EELS measurements in EM [6].

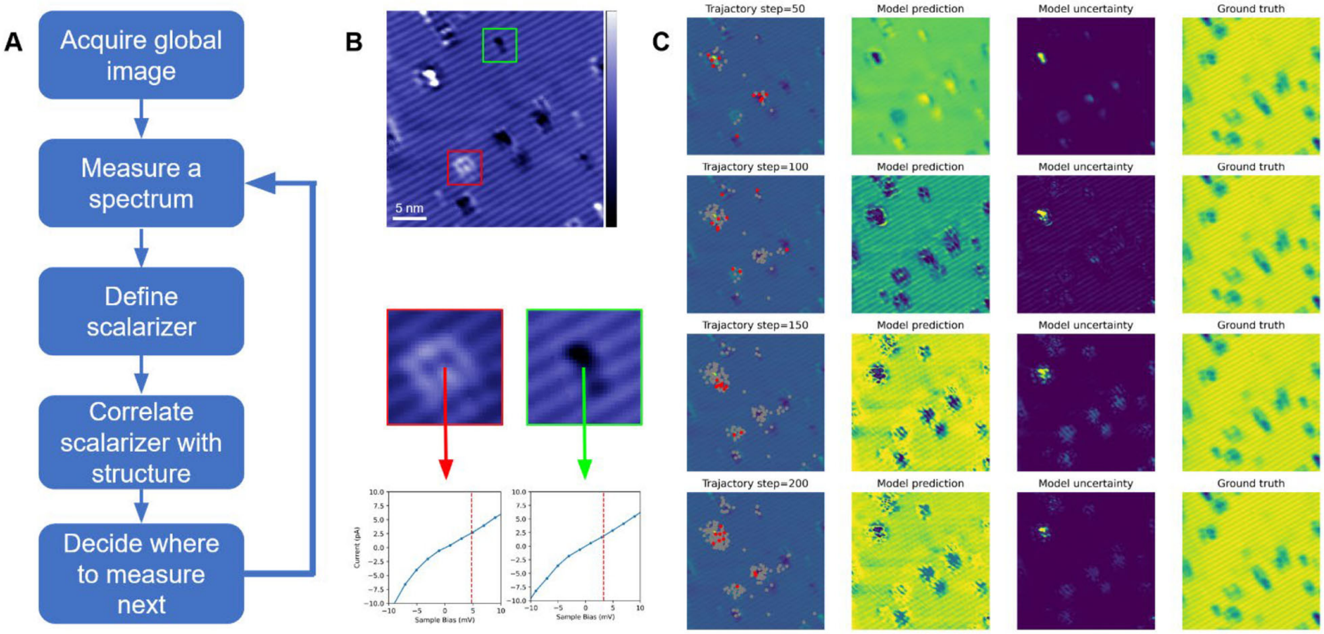

Fig. 1. A, workflow of a typical DKL experiment. **B,** the global topography image is available to the model in the beginning of the experiment. In this example of SmB6, the zero-bias, which is determined by the bias at which the tunneling current becomes zero in the I-V curve, represents the charge puddle size around impurities. DKL model learns the relationship between the zero-bias measured at a pixel and the structural patch centered at that pixel in the topography image. Then the DKL model can predict how the zero-bias look like based on the topography image with associated uncertainty. Based on **prediction**, DKL can decide where to measure the I-V curve next. **C,** a DKL simulation based on a full-grid IV measurement. From left to right: topography image, DKL prediction of zero-bias map, DKL uncertainty of zero-bias map, ground truth of zero-bias map. The gray spots in the topography map show the visited pixels in the past and red spots indicate the newly measured pixels in the latest 10 iterations. In this example, DKL can predict the zero-bias map with only 200 measurements.

References

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