Abstract Submitted
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**Machine learning and pattern recognition from surface molecular architectures.**[1] ARTEM MAKSOV, University of Tennessee, Knoxville, MAXIM ZIATDINOV, Oak Ridge National Laboratory, SHINTARO FUJII, Tokyo Institute of Technology, BOBBY SUMPTER, SERGEI KALININ , Oak Ridge National Laboratory — The ability to utilize molecular assemblies as data storage devices requires capability to identify individual molecular states on a scale of thousands of molecules. We present a novel method of applying machine learning techniques for extraction of positional and rotational information from ultra-high vacuum scanning tunneling microscopy (STM) images and apply it to self-assembled monolayer of $\pi$-bowl sumanene molecules on gold. From density functional theory (DFT) simulations, we assume existence of distinct polar and multiple azimuthal rotational states. We use DFT-generated templates in conjunction with Markov Chain Monte Carlo (MCMC) sampler and noise modeling to create synthetic images representative of our model. We extract positional information of each molecule and use nearest neighbor criteria to construct a graph input to Markov Random Field (MRF) model to identify polar rotational states. We train a convolutional Neural Network (cNN) on a synthetic dataset and combine it with MRF model to classify molecules based on their azimuthal rotational state. We demonstrate effectiveness of such approach compared to other methods. Finally, we apply our approach to experimental images and achieve complete rotational class information extraction.

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