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Application of Machine Learning tools to recognition of molecular patterns in STM images[1] ARTEM MAKSOV, UT/ORNL Bredesen Center, MAXIM ZIATDINOV, ORNL, SHINTARO FUJII, MANABU KIGUCHI, Tokyo Institute of Technology, SHUHEI HIGASHIBAYASHI, Institute for Molecular Science, HIDEHIRO SAKURAI, Osaka University, SERGEI KALININ, BOBBY SUMPTER, ORNL — The ability to utilize individual molecules and molecular assemblies as data storage elements has motivated scientist for years, concurrent with the continuous effort to shrink a size of data storage devices in microelectronics industry. One of the critical issues in this effort lies in being able to identify individual molecular assembly units (patterns), on a large scale in an automated fashion of complete information extraction. Here we present a novel method of applying machine learning techniques for extraction of positional and rotational information from scanning tunneling microscopy (STM) images of π-bowl sumanene molecules on gold. We use Markov Random Field (MRF) model to decode the polar rotational states for each molecule in a large scale STM image of molecular film. We further develop an algorithm that uses a convolutional Neural Network combined with MRF and input from density functional theory to classify molecules into different azimuthal rotational classes. Our results demonstrate that a molecular film is partitioned into distinctive azimuthal rotational domains consisting typically of 20-30 molecules. In each domain, the "bowl-down" molecules are generally surrounded by six nearest neighbor molecules in "bowl-up" configuration, and the resultant overall structure form a periodic lattice of rotational and polar states within each domain.

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