O 25: Poster Session - Focus Sessions: Innovation in Machine learning PRocEsses for Surface Science (IMPRESS)

Time: Monday 18:15–20:00 Location: P1A

O 25.1 Mon 18:15 P1A

Recovering molecular configurations during SPM-based manipulation — •Joshua Scheidt[1,2,3], Kurt Driessens[4], F. Stefan Tautz[1,2], and Christian Wagner[1,2] — [1]1Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA Fundamentals of Future Information Technology, Jülich, Germany — [3]Institut für Softwaretechnik und Theoretische Informatik, Technische Universität Berlin, Germany — [4]Department of Data Science and Knowledge Engineering, Maastricht University, The Netherlands

Molecular nanorobotics with a scanning probe microscope (SPM) would place the construction of complex supramolecular structures that are not accessible by self-assembly within reach. A fundamental obstacle on the way towards this goal is the poor observability of the atomic-scale molecular conformation during manipulation. Here we present a solution to this problem which utilises the particle filter localisation (PF) technique: Force-gradient data along a manipulation trajectory as received from the SPM is compared to data from a molecular simulation stored using a finite state automaton[1]. The simulation contains all inequivalent tip-molecule-surface configurations on a high-symmetry surface. The PF uses a set of sampling points to identify simulated conformations which likely match the experimental data. The particles from the PF are subsequently clustered to allow for a single or small set of likely molecule conformations to be retrieved. We test the performance of the PF on synthetic as well as experimentally acquired data.

[1] A. Diener, Master's thesis, Maastricht University, 2018

O 25.2 Mon 18:15 P1A

Classification of grazing incidence x-ray diffraction patterns using neural networks — •Verena Eslbauer, Johannes J. Cartus, Roland Resel, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

Grazing incidence X-ray diffraction is a frequently used tool to investigate the crystalline properties of thin films. Hereby, indexing Bragg peaks is a fundamental procedure for phase analysis and detection of unknown polymorphs. The current solution is an iterative approach, which is both tedious and requires the knowledge of an experienced material scientist. We are currently developing a software based on convolutional neural networks that should enable automatic classification of crystal systems. We have created a large set of crystal structures with pre-determined symmetries and their diffraction patterns. These serve as a training dataset for our convolutional neural network. At the current status of our work we can differentiate between different crystal systems, independent of the preferred orientation of their crystallites.

The next steps of our research involve the assignment of Laue indices to Bragg peaks and finally the determination of the lattice constants of the crystallographic unit cell.

O 25.3 Mon 18:15 P1A

Neural Network Controlled Nanocar — •Bernhard Ramsauer and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

In 2021 at the nanocar race at Center for Materials Development and Structure Studies (CEMES-CNRS) in Toulouse, France we are planning to participate with the world*s first neural-network-controlled nanocar. At this race, participants have to direct a single molecule across a 'race-track' set on a metallic substrate, controlling their nanocars via an STM-tip without being in physical contact with it.

Although nanocars can be readily synthesized with different shapes and properties, the physics that govern the molecule's movement is complex and involves the interaction between the molecule and the tip as well as between the molecule and the substrate. Therefore, it is far from straightforward for humans to manoeuvre the nanocar and predict the result of a performed action.

To improve the performance, we implement Deep Neural Networks (DNNs), which are able to perform various actions even for subsequently changing environmental conditions. The DNN enables an 'autonomous' driving of nanocars by controlling the STM-tip position and the applied voltage based on the nanocars position and orientation on the surface. Moreover, the DNNs will yield direct physical insight into the interaction that governs the nanocar maneuvers.