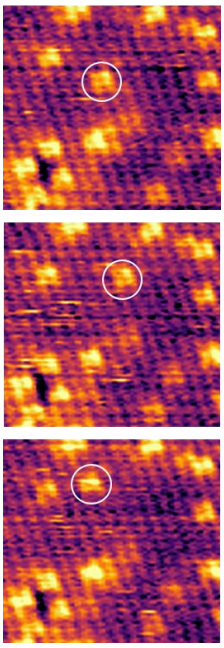
Professorship of Simulation of Nanosystems for Energy Conversion
TUM School of Computation, Information and Technology
Technische Universität München

Our research group is looking for student interested in

Master Thesis

Machine learning for tracking dynamical phenomena on atomistic resolved STM experiments



Diffusion of Fe atoms under the magnetite surface, visible as double-lobed species (circled).

The project is a collaboration between the NAT (Prof. Barbara Lechner and PD Friedrich Esch) and CIT (Prof. Alessio Gagliardi) schools. In our labs at the NAT school, we have developed we have developed an electronics add-on module for scanning probe microscopes (FastSPM) to follow dynamic processes on surfaces at the atomic scale. This method provides unique access to diffusion paths of individual atoms or particles, visualization of ongoing chemical reactions, and high spatial resolution imaging under extreme conditions. This scientific endeavor, however, requires state of the art image reconstruction from the raw data, machine learning-assisted image corrections and adequate pattern recognition to extract diffusion traces, position-dependent mobility and further quantitative information. The basic algorithms have been developed in the Python package *PyfastSPM.* In the present Master project, the successful candidate will connect *PyfastSPM* with state-of-the-art machine learning algorithms for the quantitative analysis of dynamic phenomena on surfaces. This will be done by implementing the U-Net architecture or the YOLO model. Further, if this succeeds, a time series evolution algorithm (such as LSTM, RNN or Transformers) will be trained to predict how the sites move in the matrix over time. For training and validation, several highly resolved data sets are available, such as the confined diffusion of single hydrogen atoms on an iron oxide surface. The developed methods will then be applied to scanning tunneling microscopy (STM) data sets of increasingly complex surface dynamics on the same surface, such as sub-surface iron atom diffusion or sub-nanometer metal particle dynamics.

Required Skills

Following skills would be helpful in completing the tasks of this thesis.

- Programming skills in python, pytorch.
- Familiarity with version control using Git
- Experience with or motivation to learn working with high performance computational cluster
- Basic understanding of machine learning models

Application

Write us an email at **thesis.sne@nano.cit.tum.de**

- Attach your Transcipt of Records and a CV

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