



Project – Machine learning in scanning probe microscopy

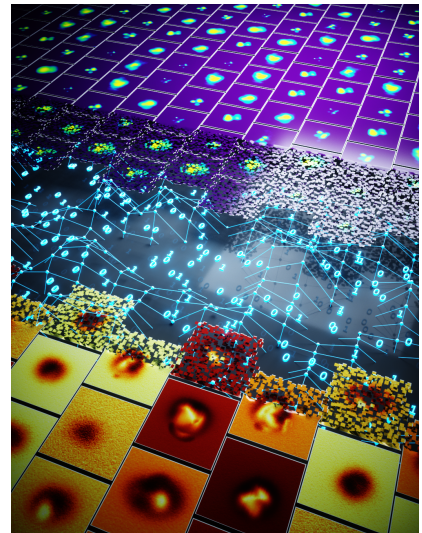


Background – Since its conception, Scanning Probe Microscopy (SPM) has led the development of the field of nanoscience, demonstrating the capability to provide atomic resolution of molecules, nanostructures, and surfaces. However, as the systems, and physics, studied have increased in complexity, the interpretation of experimental data becomes a vast, often hopeless exploration through all possible atomic configurations and imaging parameters.

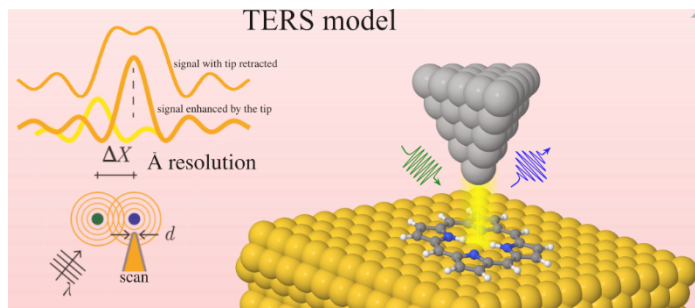
Our group has made rapid progress in the development of machine learning approaches to the simulation, analysis, and autonomous control of SPM, with applications from quantum materials to biomolecular recognition and disease classification. In this project, you will join the ML-SPM team and learn to use deep learning methods to link atomistic and quantum simulations directly to measurements.

Team – the project will be supported by our machine learning in SPM team (Lauri Kurki, Farzin Irandoost, Jie Huang, Dr. Nian Wu, Dr. Joakim Jestilä, Dr. Nan Cao).

Learn – basic ideas behind SPM and its simulation. Deep learning methodologies and applications.



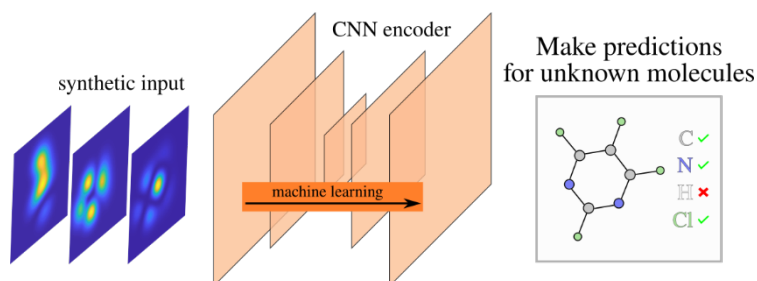
Project – Machine learning in tip enhanced Raman microscopy (TERS)



Background – Optical spectroscopy has been for ages an important characterization technique capable of providing chemical and structural information from materials in a non-destructive manner. However, due to the **Abbe diffraction limit**,

propagating light cannot be localized in a region smaller than approximately half of its wavelength. For example, the wavelength of green light is 500 nm, resulting in a spatial resolution of ~ 250 nm, way larger than typical interatomic distances. To overcome this, scientists have been illuminating samples with a light coming from a source way smaller than the typical wavelength of light, which enables them to get amazing \AA -scale resolution images. **In this project, we will focus on simulating an experiment where the light is trapped between a very sharp tip and the sample** creating a plasmonic field, which is then interpreted by a Raman spectrometer. This technique is called tip enhanced Raman spectroscopy, or TERS for short.

Our group already has made important contributions in the development of approaches within the machine learning methods to the simulation of scanning probe microscopy (SPM) images. In this project, your task will be to give the



first steps towards the development of a database of synthetic TERS images, as well as elevating our group expertise towards the implementation of machine learning approaches to prediction of structures from the TERS database.

Team – the project will be supported by quantum simulations expert (Dr. Orlando J Silveira) and our machine learning team (Lauri Kurki, Farzin Irandoost, Dr. Nian Wu, Dr. Joakim Jestilä)

Learn – basic ideas behind TERS and its simulation. Quantum simulations. Deep learning methodologies and applications.