Machine Learning tools for SPM Automation

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Machine learning (ML) has become a valuable tool for automating scanning probe microscopy (SPM) tasks such as data collection [1] and tip tuning [2]. These tasks, although routine for SPM users, can be time-consuming and complex, often requiring full supervision by a trained user. By incorporating ML techniques, we can reduce the manual workload and make SPM techniques more user-friendly and efficient.

This talk will dive into the complete workflow of developing and implementing an ML model to automate SPM tasks. Starting off with task selection where we identify what SPM procedures can benefit from automation. Then we discuss data collection and preprocessing steps taken to prepare datasets for ML model training while highlighting tools that can help with these steps. We will go over what ML models exist and how to choose a specific for a task. Following this, we will cover the training process, where the ML model learns to perform the tasks through iterative optimization. Evaluation metrics and validation techniques will be explained to ensure the model's performance meets the required standards. For each of the workflow steps this talk will provide tools and resources that can help develop these ML models.

Finally, we will demonstrate how to integrate ML models into GXSM [3], a specialized SPM software utilized at Brookhaven National Lab. The integration process will be illustrated with examples [4], showcasing how GXSM's tools facilitate the implementation of ML and automation algorithms. From this talk we demonstrate how ML methods can be implemented to automate, simplify and make SPM techniques more efficient.

References:

[1] Arias S., Zhang Y., Zahl P., Hollen S. J. Phys. Chem. A 127, 29 (2023)

[2] Rashidi M. and Wolkow R. A. ACS Nano 12 5185–9 (2018)

[3] GXSM: http://gxsm.sf.net

[4] Arias S. and Zahl P. Github repository: auto-AFM. https://github.com/pyzahl/pico-pilot