Autonomous analysis, manipulation and reactions in Scanning Probe Microscopy

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Scanning Probe Microscopy (SPM) has been the engine of characterization in nanoscale systems in general, and the evolution of functionalized tips as a reliable tool for high-resolution imaging without material restrictions has been a breakthrough in studies of molecular systems. In parallel, machine learning (ML) methods are increasingly being applied to data challenges in SPM. In particular, the success of deep learning in image recognition tasks has led to their application to the analysis of SPM images, especially in the context of surface feature characterisation and techniques for autonomously-driven SPM.

In this work, we explore the general potential for using ML approaches to aid in the analysis of Atomic Force Microscopy (AFM) and Scanning Tunnelling Microscopy (STM) images, along with the possibilities of introducing ML automation into experimental workflows. As an example, we build upon a deep learning infrastructure that matches a set of AFM/STM images with a unique descriptor characterizing the molecular configuration, and then develop a workflow that takes experimental images of complex molecular systems and revises initial ML structure predictions with neural network potential simulations [1]. In this context, we discuss the challenges of handling experimental data and possible data augmentation strategies. Beyond this, we show how ML approaches can be used actively during SPM experiments for construction of nanostructures through atomic manipulation, while also highlighting approaches towards automated construction of more complex molecular systems atom-by-atom and bond-by-bond [2].

References

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