Neural Networks in AFM

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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 [1].

In this overview, we explore the potential for using neural network based methods to aid in the analysis of high resolution Atomic Force Microscopy (AFM) images. After a basic introduction to neural networks [2], we expand into the use of Convolutional Neural Networks (CNN) for general image analysis and their particular use in AFM. Following this, we cover the basics of Graph Neural Networks (GNN) [3] and how they can be used as powerful molecular descriptors. Finally, as an example bringing everything together, we use a combination of CNN and GNN models to match a set of AFM images of ice structures with an accurate initial guess of the molecular structure. This is then revised by detailed neural network potential and quantum simulations [4].

A introductory tutorial is also offered as a homework for those wishing to build and run their own CNN on an image database.

References

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