Machine learning for Atomic Force Microscope image interpretation and device operation

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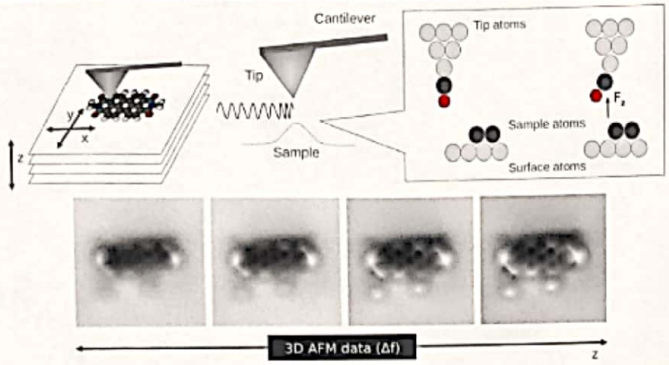
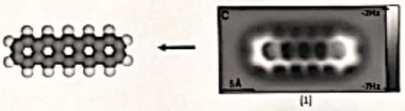
Atomic force microscopy (AFM)

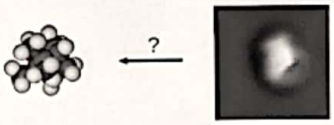


In AFM, an extremely sharp tip "touches" a sample, resulting in a force interaction that causes a deviation in the motion of the tip. A scan over the sample produces an image of the sample, and scans at different distances from the sample result in different contrast. State-of-the-art AFM devices with CO-tip functionalization can image atomic features within individual molecules on surfaces [1]. However...



[1]

..., while AFM image of flat molecules are fairly easy to interpret...

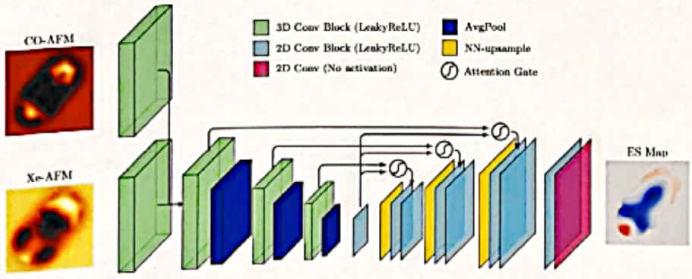


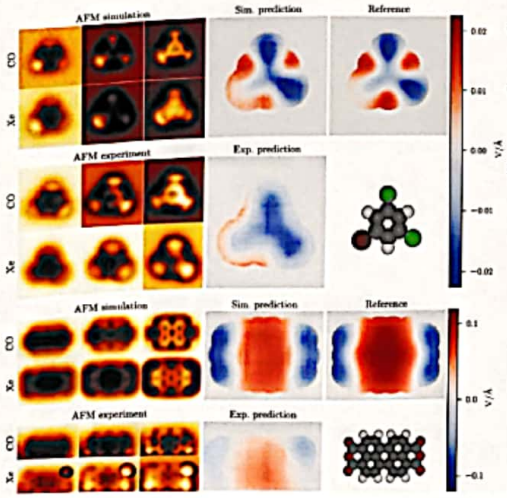
..., images of more complicated 3D geometries are much more challenging to deal with, and elemental identification is difficult in general.

Challenge: Can we recover the (partial) geometry and elements or other sample properties from the AFM image?

Sample electrostatics from AFM

The electrostatic properties of molecules play an important role in a variety of processes. We train a convolutional neural network to predict the electrostatic field at a set distance from a molecule from AFM images [4]. The model receives as inputs two sets of AFM images using two differently terminated tips, in this case CO and Xe. The different characteristic distortions resulting from different charge on the functionalized tip help give the model information about the distribution of charges on the sample.

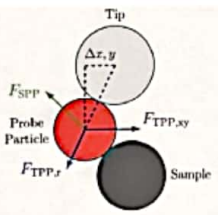


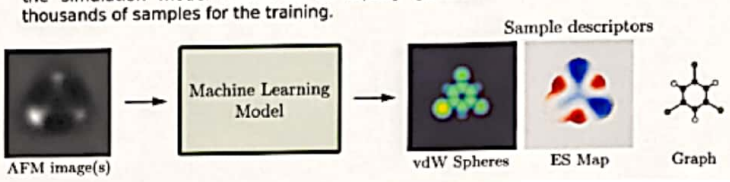


- The model has excellent accuracy on simulated test images.
- Performance is also quite good on real experimental images, but quantitative accuracy is still not reliable.
- Biggest short-coming in the current model is the use of point-charge electrostatics in the training data. We are working on changing to using more accurate DFT Hartree potentials as well as including the metallic surface in the training simulation data.

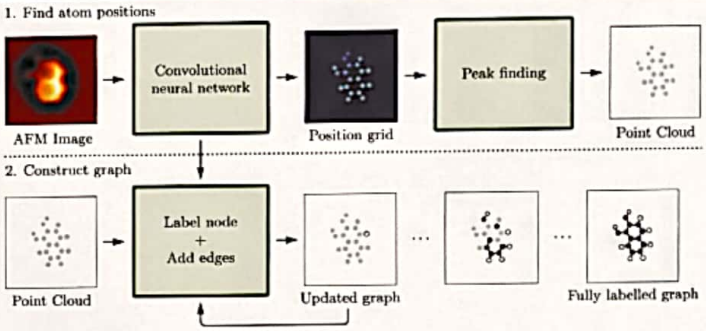
Machine learning AFM

- We have experimented on training various types of machine learning models for interpreting AFM images. The job of the model is to predict a descriptor of the sample that somehow characterizes the sample, for example the geometry or electrostatic field.
- Training the models requires a large training set of AFM images with the corresponding target descriptors. We generate the training data using simulations based on the Probe Particle Model [3]. A GPU implementation of the simulation model allows us to rapidly generate thousands of samples for the training.

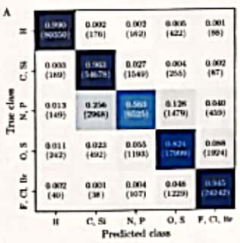


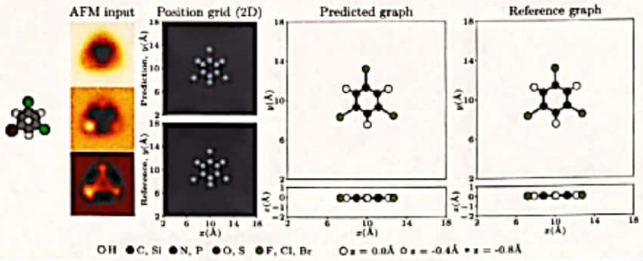


AFM images into molecule graphs



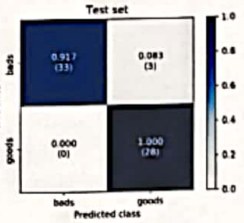
- Molecules are naturally represented as graphs of atoms and bonds.
- Graph neural networks (GNN) have recently emerged as a general framework for machine learning on graph-structured data [2]. A GNN can learn to encode the information in a molecule graph in a way that respects the inherent symmetries of the graph.
- We combine a GNN with a convolutional neural network to design a model that can be used for constructing molecule graphs from AFM images [5].

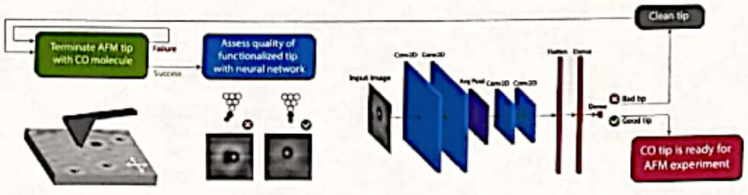




Automated tip CO-functionalization

- Tip functionalization is an essential part of the successful operation of a high-resolution AFM device. This is often a very time-consuming trial-and-error process that wastes the experimentalists' time.
- We developed a method based on convolutional neural networks for automatically assessing the quality of a CO-functionalized tip. This model is used in a fully autonomous loop that can independently repeatedly pick up a CO molecule until the functionalized tip meets the quality requirement and is ready for experiment. [6]





References

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Acknowledgements