Automated Structure Discovery in Atomic Force Microscopy

B. Alldritt[1] P. Hapala[1] N. Oinonen[1] F. Urtev[1,2] O. Krejci[1] F. F. Canova[1,3] J. Kannala[2] F. Schulz[1] P. Liljeroth[1] A. S. Foster[1,4,5]

[1]Department of Applied Physics, Aalto University, P.O. Box 11100, FI-00076 Aalto, Espoo, Finland
[2]Department of Computer Science, Aalto University, P.O. Box 11100, FI-00076 Aalto, Espoo, Finland
[3]Nanolayers Research Computing Ltd, London, UK
[4]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128, Germany
[5]WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University , Kakuma-machi, Kanazawa 920-1192, Japan

While atomically-resolved non-contact atomic force microscopy images of molecules has developed since initial reports with flexible CO and Xe terminated tips [1,2], most experiments were limited to planar molecules, due to the challenge of interpreting AFM data from non-planar molecules. Further, the interpretation of adsorption geometry of a single molecule depends on tip termination and relaxation of the tip and the sample. It is possible to simulate AFM images using a simple mechanical model [3,4], but it still requires an extensive search for a similar molecular structure that matches the experimental data. Presented are results from a combined experimental and computational investigation that suggest a convolutional neural network (CNN) trained on simulated AFM data can learn an inverse mapping process easily and identify potential geometric configurations [5]. I will discuss the results of experiments performed on 1S-camphor on a Cu(111) surface and the associ ated com putational results which led to the understanding of the geometric configurations of this molecule. This process holds significant promise for applying high-resolution AFM to a variety of systems where understanding of the chemical structure of individual molecules can be a major breakthrough.

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