

Mapping Intermolecular Force-fields with Sub-Angstrom Resolution

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Dynamic force microscopy (DFM, also called non-contact atomic force microscopy) has evolved rapidly into an exceptionally powerful tool for single molecule imaging, spectroscopy, and manipulation. A number of key innovations have enhanced the capabilities of the technique dramatically over the last decade or so: the introduction of the qPlus variant [1], facilitating exceptionally high sensitivity to short range chemical forces; the exploitation of the Pauli exclusion regime of the tip-sample interaction potential for unprecedented levels of resolution [2,3]; and the steady development of sophisticated protocols enabling greater control of the precise structure of the tip apex [2,4].

As a result of these developments, coupled with substantial support from first principles theoretical calculations such as density functional theory (DFT), DFM is now capable of not only characterising reactants and products at the single bond level [5], but of controlling bond conformation on an atom-by-atom basis [6].

I will discuss the application of qPlus DFM to the measurement of intermolecular force-fields and potential energy landscapes for three distinct classes of molecule: fullerenes (specifically, C_{60}) [7], porphyrins (tetra(4-bromophenyl)porphyrin), and NTCDI (see Fig. 1). In each case precise control of the apex of the tip is an essential prerequisite for the acquisition of quantitative force data. In the case of NTCDI this is a particularly acute issue as our primary interest lies in the measurement and exploitation of hydrogen-bonding-derived forces and potentials. Our approaches to ascertaining the chemical termination of the tip via comparison of experimental data with the results of DFT calculations will be described in some detail.

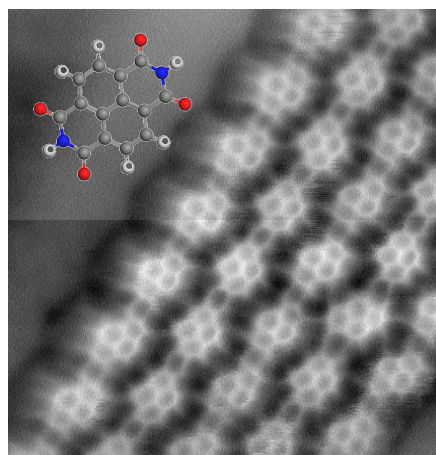


Fig. 1 qPlus DFM image of a 2D assembly of NTCDI molecules (structure shown in inset) on the Ag:Si(111)-(√3 x √3)R30° surface.

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