Combining orbital imaging with atomic resolution for tip-adsorbed molecules

Philip Moriarty
School of Physics and Astronomy,
University of Nottingham,
Nottingham NG7 2RD, UK
www.nottingham.ac.uk/physics/research/nano

Tip functionalization via the controlled transfer of an adsorbed species from a substrate has played a central role in recent remarkable advances in submolecular resolution scanning probe microscopy. In a series of pioneering experiments, Gross and coworkers [1,2] have shown that a CO-functionalized dynamic force microscope tip could be used to image the internal atomic structure of organic molecules with unprecedented resolution. Given that the contrast attained in any scanning probe microscope image is critically dependent on the tip state [3], and that single-molecule functionalization of the probe will play an increasingly important role in state-of-the-art scanning probe microscope imaging, the development of strategies to determine molecular orientation with the highest possible resolution *at the tip* is essential.

By exploiting the 'inverse imaging' technique pioneered by Giessibl and co-workers a decade ago [4], I will discuss how it is possible to ascertain the precise orientation (rotation/tilt) of a C60 molecule terminating the tip of a qPlus sensor [5]. A combination of dynamic STM (dSTM) and non-contact atomic force microscopy (NC-AFM) enables images of molecular orbital structure to be correlated with atomic resolution images. We show that not only is simple Huckel molecular orbital theory more than adequate to determine molecular orientation through comparison with experimental dSTM images but that weakly attractive tip-sample interactions are sufficient to provide atomic resolution images of the structure of the tip-adsorbed C60 cage. Thus, in this case, operation within the Pauli exclusion regime of the potential is not a prerequisite for atomic resolution NC-AFM imaging of submolecular structure.

References:

[1] L. Gross, F. Mohn, N. Moll, P. Liljeroth, and G. Meyer, Science 325, 1110 (2009).

[2] L. Gross, F. Mohn, N. Moll, G. Meyer, R. Ebel, W. Abdel-Mageed, and M. Jaspars, Nature Chem. 2, 821(2010).

[3] For a recent example, see Joachim Welker and Franz J. Giessibl, Science 336 444 (2012).

[4] F. Giessibl, S. Hembacher, H. Bielefeldt, and J. Mannhart, Science 289, 422 (2000).

[5] "Precise orientation of a single C60 molecule on the tip of a scanning probe microscope", C. Chiutu, A. M. Sweetman, A. J. Lakin, A. Stannard, S. Jarvis, L. Kantorovich, J. L. Dunn, and P. Moriarty, Phys. Rev. Lett., in press (2012).