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TÉMA

Atom manipulation and sub-molecular imaging using qPlus NC-AFM

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We present recent work investigating the mechanical manipulation of the Si(100) surface, and the determination of molecular orientation at C_{60} -functionalized tips, using a low temperature NC-AFM in the qPlus configuration. On Si(100) we show that small amplitude, zero bias NC-AFM allows for the atomically precise manipulation of the buckled dimers that form the c(4x2) surface reconstruction (Figure 1), but that the surface strain induced by defects and step edges plays a critical role in determining the energy barriers between states, and hence, the feasibility of manipulation. Following Giessibl et al.'s pioneering work on achieving "sub-atomic" contrast, we exploit the relatively large separation and narrow spatial extent of the adatom dangling bond orbitals at the Si(111)-(7x7) surface to image the apex of a C₆₀ functionalized tip, resulting in sub-molecular `inverse imaging' (Figure 2). We show that the orientation of the molecule on the apex can be determined in both NC-AFM and dynamic STM by comparison with computationally inexpensive ab inito simulations, resulting in a protocol for the creation of well defined tip apices for scanning probe experiments.



Figure 1: Manipulation of the buckled Si(100) surface by df(z) spectroscopy. A single spectroscopy point results in the correlated flip of 2 dimers – i.e. a `phason pair' is injected



Figure 2: `Inverse imaging' of a C_{60} functionalized tip on the Si(111) surface. The `5 lobe' appearance of each ad-atom reveals a `pentagon down' orientation of the C_{60} on the tip apex.

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