
**Molecules investigated
with atomic resolution
using scanning probe
microscopy with
functionalized tips**

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Single organic molecules adsorbed on ultrathin insulating films were investigated using scanning tunnelling microscopy (STM), noncontact atomic force microscopy (NC-AFM), and Kelvin probe force microscopy (KPFM). With all of these techniques submolecular resolution was obtained due to tip functionalization by atomic manipulation. The techniques yield complementary information regarding the molecular structural and electronic properties.

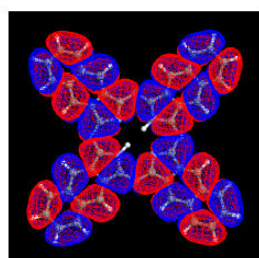
Using NC-AFM with CO terminated tips, atomic resolution on molecules has been demonstrated and the contrast mechanism was assigned to the Pauli repulsion [1]. On the other hand, by using STM the molecular frontier orbitals, i.e., the highest occupied and the lowest unoccupied molecular orbitals (HOMO and LUMO), were mapped [2]. Using a CO terminated tip for orbital imaging with the STM, the resolution can be increased and the images correspond to the gradient of the molecular orbitals due to the p-wave character of the tip states [3]. Finally, KPFM reveals information about the distribution of charges within molecules by measuring the z-component of the electrostatic field above the molecule, as demonstrated on the hydrogen tautomerization switch naphthalocyanine [4].

The possibilities of extracting additional information from AFM measurements on molecules, especially concerning intramolecular bonds, e.g. bond order and bond length, will be discussed.

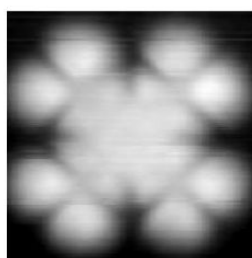
References:

- [1] L. Gross et al. Science 325, 1110 (2009)
- [2] J. Repp et al. Phys. Rev. Lett. 94, 026803 (2005)
- [3] L. Gross et al. Phys. Rev. Lett. 107, 086101 (2011)
- [4] F. Mohn et al. Nature Nanotechnol. 7, 227 (2012)

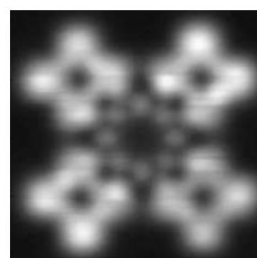
Figures:



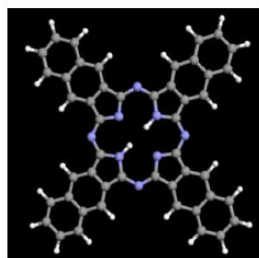
Naphthalocyanine
HOMO



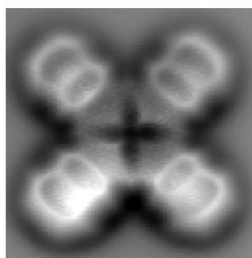
STM, Cu (**s-wave**) tip:
Orbital density [2,3]



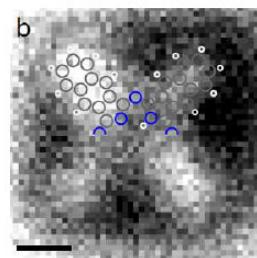
STM, CO (**p-wave**) tip:
Wave function gradient [3]



Atomic model



AFM, CO tip: Atomic
structure [1,4]



KPFM, Cu tip:
charge distribution [4]