## Individual Molecules Investigated by Scanning Probe Microscopy with Atomically Functionalized Tips

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Experiments using scanning tunneling microscopy (STM), noncontact atomic force microscopy (NC-AFM), and Kelvin probe force microscopy (KPFM) on single molecules will be reviewed. 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 functionalized tips, atomic resolution on molecules was demonstrated [1] and the technique was used to indentify unknown molecular structures [2]. Moreover, different bond orders of individual carbon-carbon bonds in polycyclic aromatic hydrocarbons and fullerenes were distinguished [3] and the exact adsorption geometry (adsorption height, site, and tilt) was measured [4]. With KPFM information about the distribution of charges within molecules was gained [5].

In particular the role of the atomic tip termination will be discussed. Mostly we used CO functionalized tips, which can enter the regime of Pauli repulsive forces and yield highly resolved images of the atoms and bonds due to tilting of the CO molecule at the tip. However, for certain investigations other tip terminations are advantageous. The choice of the best suited tip depends on the mode that is used, the property to be determined, and whether one seeks qualitative or quantitative information. Recently, we investigated additional tip functionalizations for AFM, i.e., Cl, Br, Xe, Kr, and NO [6].



**Figure:** Different scanning probe microscopy modes (STM, AFM and KPFM) using functionalized tips on a single naphthalocyanine molecule adsorbed on a double layer NaCl on Cu(111).

## References

- [1] L. Gross, F. Mohn, N. Moll, P. Liljeroth, G. Meyer, *Science* **325**, 1110 (2009)
- [2] L. Gross, F. Mohn, N. Moll, G. Meyer, R. Ebel, W. M. Abdel-Mageed, M. Jaspars, *Nature Chem.* 2, 821 (2010); K. O. Hanssen et al. *Angew. Chem. Int. Ed.* 51, 12238 (2012)
- [3] L. Gross, F. Mohn, N. Moll, B. Schuler, A. Criado, E. Guitian, D. Pena, A. Gourdon, G. Meyer, *Science* **337**, 1326 (2012)
- [4] B. Schuler, W. Liu, A. Tkatchenko, N. Moll, G. Meyer, A. Mistry, D. Fox, L. Gross, *Phys. Rev. Lett.* 111, 106103 (2013)
- [5] F. Mohn, L. Gross, N. Moll, G. Meyer, *Nature Nanotechnol.* 7, 227 (2012)
- [6] F. Mohn, B. Schuler, L. Gross, G. Meyer, Appl. Phys. Lett. 102, 073109 (2013)