

## Molecules in the transport path: The mechanical properties of STM junctions “in contact”

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In recent years, scanning tunneling microscopes (STM) have been used increasingly as devices to establish atomically defined contacts to surfaces. For the STM this has created new opportunities in various fields, ranging from quantum transport studies through nanostructures [1] to ultra-high resolution microscopy [2]. The next challenge is the combination of electrical measurements in these contacts with experiments that reveal the mechanical properties and the structure of the junction “in contact” directly. This can be achieved by equipping the tunneling microscope with a tuning fork sensor that measures the gradient of the acting force via the frequency shift of the tuning fork oscillation.

In this talk I will illustrate the benefits of combining force with current detection when molecules are in the transport path between the STM tip and the surface. Two experiments will be considered: (1) a molecular wire is lifted up between tip and surface as the tip retracts from the surface, (2) a sensor molecule is present in the tunneling junction, yielding very high lateral image resolution as the tip is scanned across the surface in near contact (scanning tunneling hydrogen microscopy, STHM).

(1) Measuring the conductance of molecular wires in well-defined geometries is still a challenge. We have shown some time ago that molecules can be contacted with an STM tip at defined positions and lifted up by tip retraction [3]. In this experiment the upper contact at the tip is defined, but for any given tip height the precise structure of the remainder of the molecule in the junction is still not known from experiment. For example, it is not clear from the conductance vs. tip height spectrum when exactly the molecule reaches the freestanding wire configuration. However, when simultaneous force detection is added, it becomes possible to determine the structure of the molecule in the junction from its mechanical response unambiguously, and in this way the intrinsic conductance of a free standing molecular wire under full structural control can be measured for the first time [4]. We have applied this to a class of conjugated molecular wires of varying lengths. Incidentally, the force gradient signal can also be used to measure the adsorption energy of a single molecule on the surface and to partition this energy between various bonding channels [5].

(2) It has been shown that atomic and molecular sensor particles in the tunneling junction lead to a dramatic enhancement of the lateral STM resolution, revealing the geometric structure of surfaces (STHM) [2]. We have suggested that this remarkable image resolution is due to force detection in the conductance channel [6]. I will show that the simultaneous detection of the force gradient signal in the tuning fork AFM and the tunneling conductance in STHM mode allows a force calibration of this conductance signal and gives further insights into the mechanism of image generation in STHM [7].

### References

- [1] C. Toher *et al.*, PRB **83**, 155402 (2011); A. Greuling *et al.*, PRB **84**, 125413 (2011); T. Brumme *et al.*, PRB **84**, 115449 (2011).
- [2] R. Temirov *et al.*, New J Phys **10**, 053012 (2008); C. Weiss *et al.*, JACS **132**, 11864 (2010); G. Kichin *et al.*, JACS **133** 16847 (2011).
- [3] R. Temirov *et al.*, Nanotechnology **19**, 065401 (2008).
- [4] N. Fournier *et al.*, PRB **84**, 035435 (2011).
- [5] C. Wagner *et al.*, PRL **109**, 076102 (2012).
- [6] C. Weiss *et al.*, PRL **105**, 086103 (2010).
- [7] G. Kichin *et al.* PRB **87**, 081408(R) (2013)