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Dr. Nikolaj Moll
IBM Research Zurich, Rüschlikon, Switzerland

“Imaging Molecules with Atomic Force Microscopy with Carbon Monoxide Terminated Tips”

Abstract:

Using functionalized tips, the atomic resolution of a single organic molecule can be achieved by noncontact atomic force microscopy (nc-AFM). The source of the high resolution is Pauli repulsion, whereas van-der-Waals and electrostatic forces only add a diffuse attractive background.

We propose a simple model in which the Pauli repulsion is assumed to follow a power law as a function of the probed charge density. The exponent in this power law is found to be largely independent of the sample molecule. The van-der-Waals and electrostatic forces are added to obtain the full tipample interactions. Our model provides a general method for simulating atomically resolved AFM images of organic molecules. It eliminates the need to take into account the full tip and sample system and therefore dramatically reduces computational cost.

The tilting of the CO at the tip is studied in detail. The tilt is induced by van-der-Waals forces, enlarges the apparent size of parts of the molecule by up to 50%. Moreover, the CO tilting in response to local Pauli repulsion causes a significant sharpening of the molecule bonds in AFM imaging. With these image distortions it is possible to distinguish different bond orders of individual carbon-carbon bonds in organic molecules by AFM.

With atomic manipulation techniques we induce a on-surface transformation of an individual aromatic molecule into a highly strained 1C-membered ring. The formation and breaking of the C–C bond is reversible which opens up the entire field of radical chemistry for on-surface reactions by atomic manipulation.

Gastgeber: Prof. Dr. Franz Gießibl