Imaging Atoms and Bonds by Atomic Force Microscopy

Nikolaj Moll, Leo Gross, Bruno Schuler, Fabian Mohn, Alessandro Curioni, and Gerhard Meyer

IBM Research – Zurich, Säumerstrasse 4, CH-8803 Ruschlikon, Switzerland

Using functionalized tips, the atomic resolution of a single organic molecule can be achieved by noncontact atomic force microscopy (nc-AFM) operating in the regime of short-ranged repulsive Pauli forces. The van-der-Waals and electrostatic interactions only add a diffuse attractive background and do not contribute to atomic contrast. To theoretically describe the atomic contrast in such AFM images, a simple model is proposed in which the Pauli repulsion is assumed to follow a power law as a function of the probed charge density. For a single molecules imaged with a CO-terminated tip, we find excellent agreement with the experimental data. Experimentally, different bond orders of individual carbon-carbon bonds in organic molecules can be distinguished by AFM with a CO-terminated tip. Two different contrast mechanisms exist, which were corroborated by calculations: The greater electron density in bonds of higher bond order led to a stronger Pauli repulsion, which enhanced the brightness of these bonds in high-resolution AFM images. The apparent bond length in the AFM images decreased with increasing bond order because of tilting of the CO molecule at the tip apex.

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