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Image Distortions of Molecules in Atomic Force Microscopy with Carbon Monoxide Terminated Tips NIKOLAJ MOLL, LEO GROSS, BRUNO SCHULER, ALESSANDRO CURIONI, GERHARD MEYER, IBM Research - Zurich — Using functionalized tips, the atomic resolution of a single organic molecule can be achieved by atomic force microscopy (AFM) operating in the regime of short-ranged repulsive Pauli forces while the van-der-Waals and electrostatic interactions only add a diffuse attractive background¹. The underlying mechanisms of image distortions with CO-terminated tips are identified and studied in detail². Parts of a molecule appear different in size, which primarily originates from the charge density. Further, tilting of the CO at the tip, 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.

¹L. Gross, F. Mohn, N. Moll, P. Liljeroth, and G. Meyer, *Science* 325, 1110 (2009).

²N. Moll, B. Schuler, S. Kawai, F. Xu, L. Peng, A. Orita, J. Otera, A. Curioni, M. Neu, J. Repp, G. Meyer, and L. Gross, *Nano Lett.* (2014).

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