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Molecular Geometry Determination by Atomic Force Microscopy NIKOLAJ MOLL, LEO GROSS, BRUNO SCHULER, FABIAN MOHN, 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 background.[1] To theoretically describe the atomic contrast a simple model is introduced in which the Pauli repulsion is assumed to follow a power law as a function of the probed charge density. Even, different bond orders of individual carbon-carbon bonds in organic molecules can be distinguished by AFM.[2] The adsorption geometry of single molecules with intramolecular resolution were measured. The lateral adsorption position was determined with atomic resolution, adsorption height differences, and tilts of the molecular plane with very high precision.[3]

[1]L. Gross, F. Mohn, N. Moll, P. Liljeroth, and G. Meyer, Science 325, 1110 (2009).
[2]L. Gross, F. Mohn, N. Moll, B. Schuler, A. Criado, E. Guitián, D. Peña, A. Gourdon, and G. Meyer, Science 337, 1326 (2012).
[3]B. Schuler, W. Liu, A. Tkatchenko, N. Moll, G. Meyer, A. Mistry, D. Fox, and L. Gross, Phys. Rev. Lett. 111, 106103 (2013).

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