O 15: STM/AFM: New Approaches

Time: Monday 15:00–18:30 Location: H24

O 15.1 Mon 15:00 H24

Imaging Molecules in Atomic Force Microscopy with Carbon Monoxide Terminated Tips — •Nikolaj Moll, Leo Gross, Niko Pavliček, Bruno Schuler, and Gerhard Meyer — IBM Research – Zurich, Säumerstrasse 4, CH-8803 Rüschlikon, Switzerland

Using functionalized tips, the atomic resolution of a single organic molecule can be achieved by atomic force microscopy (AFM). We operate in the regime of short-ranged repulsive Pauli forces while the van-der-Waals and electrostatic interactions only add a diffuse attractive background. With atomic manipulation techniques we induce a on-surface transformation of an individual aromatic molecule into a highly strained 10-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.

O 15.2 Mon 15:15 H24

Sub-molecular imaging by NC-AFM with an oxygen atom rigidly connected to a metallic probe — Oscar Díaz Arado[1], •Harry Mönig[1], Diego Rodríguez Hermoso[2], Milica Todorevic[2], Alexander Timmer[1], Simon Schüer[1], Gernot Langewisch[1], Rubén Pérez[2], and Harald Fuchs[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain

In scanning probe microscopy, the imaging characteristics in the various interaction channels crucially depend on the chemical termination of the probe tip. Here we analyze the contrast signatures of an O-terminated Cu tip with a tetrahedral configuration of the covalently bound terminal O atom. Supported by first-principles calculations, NC-AFM, and STM experiments, we show how this tip can be identified on a partially oxidized Cu(110) surface. After controlled tip functionalization, constant height NC-AFM imaging in the repulsive force regime reveals the internal bond structure of an organic molecule. In established tip functionalization approaches, the probe particles (e.g. CO or Xe) are only weakly bound to the metallic tip leading to lateral deflections during scanning. In contrast, our simulations for our tip show that lateral deflections of the terminating O atom are negligible. Its structural rigidity, chemically passivated state and a high electron density at the apex make the O-terminated Cu tip a highly attractive complementary probe for the characterization of organic nanostructures on surfaces.

O 15.3 Mon 15:30 H24

Influence of tip sharpness on subatomic resolution capability of atomic force microscopy — •Julian Berwanger, Ferdinand Huber, and Franz Josef Giessibl — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

By lateral manipulation, we show that the predicted diffusion barrier of 28.5meV of a single iron adatom [1] is lowered due to the presence of the tip by about 70% [2] and that the force responsible for manipulation is purely attractive for both Cu-terminated and CO-terminated tips. Moreover, we find that the metallic background of the functionalized tips strongly influences the tip-adatom interaction and the appearance of adatoms in the AFM channel. In a pyramidical tip model an increase of the apex angle from 126.0° to 126.9° already change the tip-adatom interaction from purely attractive to preferably repulsive. The tip with the apex angle of 126.0° can image adatoms at a by 30pm reduced tip-sample-distance compared to the tip with an apex angle of 126.9°. Subatomic resolution can only be obtained at relatively close tip-sample distances. Therefore we suggest that only "sharp" CO-terminated tips allow subatomic resolution [3]. [1] N. N. Negulyaev et al. PRB 79, 195411 (2009), [2] M. Emmrich et al. PRL 114, 146101 (2015), [3] M. Emmrich et al. Science 348, 308 (2015)

Invited Talk O 15.4 Mon 15:45 H24

Exploring chemical properties of surfaces by means of Atomic Force Microscopy — •Pavel Jelinek — Institute of Physics of the CAS, Cukrovarnicka 10, Praha, Czech Republic

Atomic resolution and manipulation is routinely achieved by both scanning tunneling microscopy (STM) and atomic force microscopy (AFM) nowadays. Despite of large activities in development of the technique, still some challenges remain, namely the chemical sensitivity on atomic level. It was demonstrated that AFM force spectroscopy could provide chemical identity of single atoms [1,2]. In this talk we present two novel methods extending further the chemical sensitivity of AFM. Electronegativity has been an important concept in chemistry, originally defined by Pauling as 'the power of an atom in a molecule to attract electrons to itself'. However its experimental determination is very limited. We present a new methodology to measure Pauling's electronegativity of individual atoms on surfaces by atomic force microscopy (AFM). Secondly we show that molecular recognition can be achieved using an analysis of characteristic minima (z_{min}(x,y) and df_{min}(x,y)) of 3D high-resolution maps combined with theoretical modeling.

[1] Y. Sugimoto et al Nature 446, 64 (2007) [2] M. Setvin et al ACS Nano 6, 6969 (2012)

O 15.5 Mon 16:15 H24

Atomic force microscopy reveals the structure of its tip and subatomic resolution on single iron adatoms — Matthias Emmrich[1], •Ferdinand Huber[1], Florian Pielmeier[1], Joachim Welker[1], Thomas Hofmann[1], Maximilian Schneiderbauer[1], Daniel Meuer[1], Svitlana Poleysa[2], Sergiy Mankovsky[2], Diemo Ködderitzsch[2], Hubert Ebert[2], and Franz J. Giessibl[1] — [1]Institute of Experimental and Applied Physics, Department of Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Department Chemie, Ludwig-Maximilians-Universität München, Butenandtstraße 11, 81377 München, Germany

A CO molecule adsorbed on a Cu(111) surface can be used to probe the apex of an atomic force microscopy (AFM) tip [1]. In our recent work [2], we invert our previous experiment [1] and functionalize our tip with a CO molecule [3] to investigate single adatoms and clusters built from individual iron atoms adsorbed on a Cu(111) surface. Our findings correct our previous interpretation [1] and suggest that dual and triple minima in the force signal are caused by dimer and trimer tips, respectively [2]. However, we show subatomic resolution AFM: single iron adatoms do not appear as a single depression or protrusion, but as a toroidal structure. Its shape reflects the bonding symmetry of the adatom to the underlying substrate. Density functional theory (DFT) calculations support the experimental data.

[1] J. Welker and F. J. Giessibl, Science **336**, 444 (2012)
[2] M. Emmrich, F. Huber *et al.*, Science **348**, 308 (2015)
[3] L. Gross *et al.*, Science **325**, 1110 (2009)

O 15.6 Mon 16:30 H24

High-resolution AFM/STM imaging and force spectroscopy of van der Walls nanostructures on metal surface — •Martin Svec[1], Oleksander Stetsovych[1], Jan Berger[1], Pavel Hobza[2], and Pavel Jelinek[1] — [1]Institute of Physics AS CR, Prague, CZ — [2]Institute of Organic Chemistry and Biochemistry AS CR, Prague, CZ

Proper theoretical description of the weak vdW interaction, despite the large effort, still remains elusive and is intensely investigated. We prepared and investigated vdW nanostructures made of CO and Xe co-deposited on Ag(111) surface by a high-resolution 3D mapping with the AFM technique. We identify the atomic structure of such formations. In addition, we use the force-distance spectroscopy data, acquired with functionalized (CO, Xe) tips to gain direct access to the vdW forces acting between two well-defined systems. Such information provides a unique opportunity to benchmark the available theoretical methods employed to describe the vdW interaction. We will provide a direct comparison of various vdW methods to the experimental data.

O 15.7 Mon 16:45 H24

Intramolecular force contrast and dynamic current-distance measurements at room temperature — •Sonia Matencio[1,2], Ferdinand Huber[1], Alfred J. Weymouth[1], Carmen Ocal[2], Esther Barrena[2], and Franz J. Giessibl[1] — [1]Department of Physics, University of Regensburg, Germany — [2]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

AFM can be used to probe the internal atomic structure of molecules [1]. Intramolecular resolution requires an unreactive tip and has been achieved at low temperatures. In the presented work we demonstrate intramolecular and intermolecular force contrast at room temperature on PTCDA molecules adsorbed on a Ag/Si(111)$-\sqrt{3}\times\sqrt{3}$ surface [2].

In addition, the oscillating force sensor allows us to dynamically measure the vertical decay constant of the tunneling current, κ [3]. The precision of the κ measurement was increased by quantifying the transimpedance of the current to voltage converter and accounting for the tip oscillation. The obtained κ maps show contrast between the two non equivalent PTCDA molecules of the herringbone phase giving evidence of a different tunneling barrier height.

[1] L. Gross et al. Science 325, 1110 (2009).

[2] F. Huber, S. Matencio et al. Phys. Rev. Lett. 115, 066101 (2015).

[3] M. Herz et al. Appl. Phys. Lett. 86, 153101 (2005); G. Binnig et al. Surf. Sci. 126, 236 (1983).

O 15.8 Mon 17:00 H24

Sub-molecular resolution imaging of molecules by AFM: Pauli versus Coulomb — Joost van der Lit[1], •Nadine J. van der Heijden[1], Francesca Di Cicco[1], Prokop Hapala[2], Pavel Jelinek[2], and Ingmar Swart[1] — [1]Condensed Matter and Interfaces, Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, The Netherlands — [2]Institute of Physics, Academy of Sciences, Prague, Czech Republic

In the past year, the origin of the contrast mechanism responsible for sub-molecular resolution imaging of molecules with functionalized tips has been a point of great discussion [1-3]. Especially the flexibility of the probe contributes to the high spatial resolution. Initially, van der Waals and Pauli interactions were thought to be responsible for the tip bending. Recently, it has been realized that also electrostatic forces influence the contrast [4]. Here, we study the role of the electrostatic force on the tip by imaging strongly polarized molecules with differently polarized tips. The charge on the final atom of the tip can be varied by different tip termination. CO tips yield nearly neutral tips while Xe terminated tips have a slight positive charge. This results in a difference in contrast in the final AFM image. References: [1] P. Hampala, PRB, 80, 085421, (2014). [2] J. Zhang, Science, 342, 611, (2013). [3] S. Hämäläinen, Phys. Rev. Lett. 113, 186102 (2014). [4] P. Hapala, Phys. Rev. Lett. 113, 226101 (2014).

O 15.9 Mon 17:15 H24

Extending carbon monoxide front atom identification (COFI) to probe the second atomic layer of an AFM tip — •Daniel Meuer, Andreas Bartholomäus Kelbel, and Franz Josef Giessibl — Universität Regensburg, Germany

The structural details of the tip determine the spatial resolution and the contrast which is obtained in atomic force microscopy. Welker and Giessibl demonstrated, that a CO molecule on a Cu(111) surface can characterize the foremost atomic layer of the apex of a metallic tip [1]. A detailed knowledge of the second atomic layer of the tip would allow even more insights into the tip structure.

In COFI, the upright bonded CO molecule on, e.g. Cu(111) probes the front atoms of the tip. We present a new technique where we put a CO on a Cu adatom essentially lengthening the CO molecule to a CuCO molecule. Then we trace the tip along a bell shaped curve to be closer to the second layer atoms next to the front most atoms. This method, which we call CuCOFI, allows us to characterize even the second atomic layer of the tip apex in situ by AFM.

References: [1] J. Welker and F. J. Giessibl, Science 336, 444 (2012)

O 15.10 Mon 17:30 H24

Understanding high-resolution AFM images of water clusters on NaCl substrate — •Prokop Hapala[1], Jing Guo[2], Jinbo Peng[2], Duanyun Cao[2], Limei Xu[2], Enge Wang[2], Ying Jiang[2], and Pavel Jelinek[1] — [1]Institute of Physics , Academy of Sciences of the Czech Republic, Cukrovarnická 10, Prague, 16253, Czech Republic — [2]International Center for Quantum Materials (ICQM) and School of Physics, Peking University, Beijing 100871, China

AFM using functionalized tips not only reveals chemical bonds within molecules [1], but it is also an ideal tool for sensing of non-covalent interactions. Recently we uncovered, using our molecular mechanics model [2], a crucial importance of electrostatic interaction in AFM images of various polar molecules [3]. In this talk we will show that the AFM imaging of water clusters formed on NaCl surface [4] is also governed by electrostatic field originating from both the polar O-H bonds and the ionic surface. The theoretical and experimental comparison between CO and Cl modified tip indicate that chiral pattern observed with negatively charged Cl tip is predominantly due to electrostatics. The ability to acquire and understand high-resolution AFM images of weakly bonded systems opens new possibilities of AFM in supramolecular chemistry and biochemistry. 1. Gross, L. et, al. Science 325, 1110-1114 (2009). 2. Hapala, P. et al. Phys. Rev. B 90, 085421 (2014). 3. Hapala, P. et al. (2015) (submitted) 4. Guo, J. et al. Nat. Mater. 13, 184-9 (2014).

O 15.11 Mon 17:45 H24

Scanning quantum dot microscopy made faster — •Christian Wagner[1,2], Michael Maiworm[3], Christian Müller[3], Matthew F. B. Green[1,2], Philipp Leinen[1,2], Eric Bullinger[3], Rolf Findeisen[3], F. Stefan Tautz[1,2], and Ruslan Temirov[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Institute for Automation Engineering (IFAT), Otto-von-Guericke University Magdeburg, Germany

Scanning quantum dot microscopy (SQDM) is a novel NC-AFM based scanning probe method that allows for the measurement of electric potentials with high sensitivity and spatial resolution[1]. To record SQDM images a single organic molecule is attached to the probe tip. This sensor molecule works as a quantum dot that can be charged via tunneling to or from the tip, depending on the local electrostatic potential. In a $\Delta f(V)$ spectrum the charging event causes a sharp dip, the position of which is the actual quantity of interest. The sharpness of this dip ($\approx$ 30 meV) suggests that methods beyond $\Delta f(V)$ spectroscopy could be used to measure its position, allowing image acquisition time to decrease from hours to minutes, making the method more versatile and easy to use. We discuss an approach to this task that is based on concepts from control theory such as system identification and extremum seeking controller.

[1] C. Wagner, M.F.B. Green, P. Leinen, T. Deilmann, P. Krüger, M. Rohlfing, R. Temirov, and F.S. Tautz, *Phys.Rev.Lett.* **115**, 026101 (2015).

O 15.12 Mon 18:00 H24

The energy resolution function of a tunnel junction — •Christian R. Ast[1], Berthold Jäck[1], Jacob Senkpiel[1], Matthias Eltschka[1], Markus Etzkorn[1], Joachim Ankerhold[2], and Klaus Kern[1,3] — [1]MPI für Festkörperforschung, 70569 Stuttgart — [2]Institut für Komplexe Quantensysteme and IQST, Universität Ulm, 89069 Ulm — [3]ICMP, EPFL, 1015 Lausanne, Switzerland

The tunnel junction between tip and sample in a scanning tunneling microscope is an ideal platform to access the local density of states in the sample through the differential conductance. We show that the energy resolution that can be obtained is principally limited by the electromagnetic interaction of the tunneling electrons with the surrounding environmental impedance as well as the capacitative noise of the junction. The parameter tuning the sensitivity to the environmental impedance is the capacitance of the tunnel junction. The higher the junction capacitance, the less sensitive the tunnel junction to the environment resulting in better energy resolution. Modeling this effect within P(E)-theory, the P(E)-function describes the probability for a tunneling electron to exchange energy with the environment and can be regarded as the resolution function of the tunnel junction. We experimentally demonstrate this effect in a scanning tunneling microscope with a superconducting aluminum tip and a superconducting aluminum sample at a base temperature of 15 mK, where it is most pronounced.

O 15.13 Mon 18:15 H24

Scanning Tunneling Microscopy at 20 mK — •Timofey Balashov, Michael Meyer, and Wulf Wulfhekel — Physikalisches Institut, KIT, Karlsruhe, Germany

We present a compact experimental setup for scanning tunneling microscopy and spectroscopy at 20 mK. To achieve this temperature, the microscope is mounted in a bath cryostat containing a ^{3}He/^{4}He dilution system. High mechanical stability and low electronic noise ensure a high energy resolution below 50 μeV. Additional capabilities include a 6 T axial magnetic field, quick tip and sample exchange and deposition of materials at low temperatures.

The high energy resolution enables precise measurements of complicated electronic systems and inelastic excitations. To demonstrate the capabilities of the instrument, we show measurements of magnetic excitations of Fe atoms on Pt(111).