

## O 15: Scanning Probe Techniques: STM/AFM

Time: Monday 15:00–18:15

Location: MA 043

O 15.1 Mon 15:00 MA 043

**Switching a four-atom Si quantum dot with the tunneling current and atomic force by means of scanning probe microscopy**— SHIRO YAMAZAKI<sup>1</sup>, KEISUKE MAEDA<sup>1</sup>, YOSHIKI SUGIMOTO<sup>1</sup>, MASAYUKI ABE<sup>1</sup>, VLADIMIR ZOBAC<sup>2</sup>, PABLO POU<sup>3</sup>, LUCIA RODRIGO<sup>3</sup>, PINGO MUTOMBO<sup>2</sup>, RUBEN PEREZ<sup>3</sup>, ●PAVEL JELINEK<sup>1,2</sup>, and SEIZO MORITA<sup>1</sup> — <sup>1</sup>Osaka University, Japan — <sup>2</sup>Institute of Physics of the CAS, Prague, Czech Republic — <sup>3</sup>Universidad Autonoma de Madrid, Spain

Most of present switching mechanisms employ the electronic excitation using scanning tunneling microscopy (STM). But only few realizations of mechanical switches using non-contact atomic force microscopy (NC-AFM) have been reported so far. Here we show that simultaneous combination of the tunneling current (STM) and atomic force (AFM) provides new possibilities to control atomic configuration of nanostructures. First we use atomic manipulation to engineer bi-stable silicon quantum dot (QD) consisting of four buckled atoms on the Si(111)-7x7 surface. We show that application of the force and the current induces the opposite upward and downward switching of atoms in the Si4-QD. This allows us to perform controlled switching between different logical states of Si-QD by the tunneling current and/or the force. What more, simultaneous application of the current and force allows us controlling switching rates. We believe that selective application of two different mechanisms opens new horizons for nanoscale switching devices or atomic manipulation.

O 15.2 Mon 15:15 MA 043

**Quantifying the virtual ground of a STM pre-amplifier**

— ●NIRMALESH KUMAR SAMPATH KUMAR, ALFERD J WEYMOUTH, and FRANZ J GIESSIBL — Institute of Experimental and Applied Physics, University of Regensburg, Universitatstraße 31, 93053 Regensburg, Germany

In AFM, it is normal to apply a bias voltage between the tip and the sample, most often to compensate for the contact potential difference. In order to perform simultaneous STM, the tunneling current must be measured. This usually involves a preamplifier that holds its current input terminal at a virtual ground that is ideally equal to real ground. Limitations of amplifier bandwidth, gain and slew rate lead to time-dependent deviations of virtual ground from zero, causing a time-dependent variation of the electrostatic force between tip and sample. These time-dependent deviations can lead to artifacts in apparent dissipation and even to an apparent "self" excitation of the cantilever. Here, we monitor virtual ground and discuss the effect of virtual ground deviations to apparent dissipation.

O 15.3 Mon 15:30 MA 043

**Atomic-scale dissipation in atomic force microscopy imaging of TlBiSe<sub>2</sub>**

— ●FLORIAN PIELMEIER, JULIAN BERWANGER, and FRANZ J GIESSIBL — Institut für Experimentelle und Angewandte Physik der Universität Regensburg, 93053 Regensburg, Deutschland

The surface termination of cleaved TlBiSe<sub>2</sub>(111) was recently studied by scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) [1,2]. Both methods revealed the unusual termination of the surface which is composed of hexagonally ordered Tl islands. Besides the atomic resolution in the frequency shift signal of our cantilever we also observe a distinct atomic-scale dissipation signal on the order of 10 meV/cycle. The dissipation is reduced at the atomic sites which are surrounded by a ring of increased dissipation. We attribute the ring-like structure of the dissipation pattern to lateral jumps of the weakly bonded Tl atoms of the surface. [1] K. Kuroda et al., Phys. Rev. B 88, 245308 (2013), [2] F. Pielmeier et al., submitted.

O 15.4 Mon 15:45 MA 043

**3D visual feedback during molecular manipulation**— ●PHILIPP LEINEN<sup>1,2</sup>, MATTHEW F. B. GREEN<sup>1,2</sup>, TANER ESAT<sup>1,2</sup>, CHRISTIAN WAGNER<sup>1,2</sup>, F. STEFAN TAUTZ<sup>1,2</sup>, and RUSLAN TEMIROV<sup>1,2</sup> — <sup>1</sup>Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — <sup>2</sup>JARA-Fundamentals of Future Information Technology

The scanning probe microscope is the tool of choice for the manipulation of single molecules on surfaces. With increased molecular complexity the number of degrees of freedom of such systems increases likewise. The respective high-dimensional potential energy surfaces

call for the use of customized tip-trajectories for successful manipulation. Here, we present an intuitive approach to the task of SPM-based manipulation of large organic molecules. In brief, we connect a motion tracking and a 3D visualization device to a low-temperature non-contact atomic force microscope / scanning tunneling microscope (nc-AFM/STM). As a proof of principle application we demonstrate the controlled removal of single molecules from a monolayer of 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA). The mutual hydrogen bonds in such a layer can only be broken if a specific tip-trajectory is used [1]. The motion tracker allows to find such a trajectory within minutes in a trial and error approach. Using immersive 3D glasses we provide the experimenter with a visualization of the current as well as previous tip trajectories and thus allow a systematic search by selective variation.

[1] M. F. B. Green, T. Esat, C. Wagner, P. Leinen, A. Grötsch, F. S. Tautz, and R. Temirov, *Beilstein J. Nanotechnol.* **5**, 1926 (2014).

O 15.5 Mon 16:00 MA 043

**3-D force and current mapping on PTCDA/Ag(111): the effect of inherent charge at the probe Xe atom**— ●OLEKSANDR STETSOVYCH<sup>1</sup>, PROKOP HAPALA<sup>1</sup>, ONDŘEJ KREJČÍ<sup>1</sup>, MARTIN ONDRÁČEK<sup>1</sup>, MARTIN ŠVEC<sup>1</sup>, and PAVEL JELÍNEK<sup>1,2</sup> — <sup>1</sup>Institute of Physics, ASCR, Praha, Czech Republic — <sup>2</sup>Graduate School of Engineering, Osaka University, Japan

The combination of STM and dynamic AFM with functionalized tips allows the investigation of structural and electronic properties of organic molecules with high resolution. In this work, we employ Kolibri sensor with Xe-functionalized tip to acquire simultaneous 3D maps of the force, tunneling current and dissipation over the PTCDA deposited on Ag(111). The detailed contrast features of the force maps at various tip-sample separations are compared to a numerical model. The model describes relaxation of the Xe atom on the probe due to Pauli repulsion and electrostatic interaction with the surface.

Moreover, we observe a specific contrast difference between two independent measurements with Xe-functionalized tips. With a support of the model, it is possible to attribute the varying contrast to an inherent charge on the Xe-atom probe. By a careful comparison of the experimental and simulated data, we can analyze the electrostatic forces acting between the tip and molecule.

O 15.6 Mon 16:15 MA 043

**Chemical identification of atoms in an organic molecule using high-resolution atomic force microscopy**— ●NADINE JACOB VAN DER HEIJDEN<sup>1</sup>, PROKOP HAPALA<sup>2</sup>, JEROEN ROMBOUTS<sup>3</sup>, JOOST VAN DER LIT<sup>1</sup>, PINGO MUTOMBO<sup>2</sup>, PAVEL JELINEK<sup>2</sup>, and INGEMAR SWART<sup>1</sup> — <sup>1</sup>Condensed Matter and Interfaces, Utrecht University, The Netherlands — <sup>2</sup>Institute of Physics of the Czech Academy of Science, Prague, Czech Republic — <sup>3</sup>VU University, Amsterdam, The Netherlands

Scanning probe techniques, such as scanning tunneling microscopy (STM) and atomic force microscopy (AFM), can provide detailed information about the geometric and electronic structure of surfaces and molecules with atomic spatial resolution. However, current methods lack one important capability essential to realize the full potential of these techniques in molecular electronics and chemistry: sensitivity towards element, valence and functional group.

Here, we show that AFM combined with force-distance spectroscopy (FDS) and theoretical calculations can be used to achieve this goal. The central idea is that the force versus distance spectra depend on the chemical nature of the atom atop of which the spectrum is acquired. By acquiring a 3D force grid over a model molecule, we demonstrate that chemical sensitivity can indeed be obtained.

O 15.7 Mon 16:30 MA 043

**Force Field Analysis of STM/AFM Tips for Atomic Manipulation**

— MATTHIAS EMMRICH, MAXIMILIAN SCHNEIDERBAUER, ●FERDINAND HUBER, ALFRED JOHN WEYMOUTH, and FRANZ JOSEF GIESSIBL — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Atomic manipulation of single atoms and molecules by scanning tunneling microscopy (STM) relies on the force field the tip exerts on the adsorbate that is to be moved. We use combined STM and atomic force

microscopy (AFM) operating at low temperature to analyze the force field between metallic tips and a CO molecule adsorbed on a Cu(111) surface [1]. We relate the force field of the tip to its suitability for reliable atomic manipulation and we find that the STM channel alone can lead to incorrect identifications of the pushing, pulling and sliding modes that have previously been identified. Circularly symmetric tips, obtained by poking, yield the most reliable manipulation. The symmetry of the force field can be assessed indirectly by evaluation of the manipulation pattern in the STM channel. In the first publication on manipulation forces [2], a lateral force of  $160 \pm 30$  pN has been measured to move CO across Cu(111) at a temperature of 5 K. Here, we find that 96 pN suffices at a temperature of 7.5 K, suggesting that thermal excitation assists atomic manipulation.

[1] M. Emmrich, M. Schneiderbauer, F. Huber, A. J. Weymouth and F. J. Giessibl, *submitted* (2014)

[2] M. Ternes, C. P. Lutz, C. F. Hirjibehedin, F. J. Giessibl and A. J. Heinrich, *Science* **319**, 1066 (2008)

O 15.8 Mon 16:45 MA 043

**Mapping intra-molecular charge distribution by distortions in high-resolution AFM/STM microscopy** — ●PROKOP HAPALA<sup>1</sup>, MARTIN ONDRACEK<sup>1</sup>, STEFAN TAUTZ<sup>2</sup>, RUSLAN TEMIROV<sup>2</sup>, and PAVEL JELINEK<sup>1</sup> — <sup>1</sup>Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, Prague, 16253, Czech Republic — <sup>2</sup>Institut für Bio- und Nanosysteme 3, Forschungszentrum Jülich, 52425 Jülich

Distribution of electron charge in molecules is a central property for chemistry since it indicates nature of bonding. Ionic bonds, polar covalent and non-polar covalent bonds of different bond order distinguish from each other by different charge distribution. At the same time, the internal charge transfer in molecules caused by presence of atoms with different electronegativity can help with identification of these atoms. In this work, we extend our simple mechanical model [1] for simulation of high-resolution AFM and STM images by incorporation of electrostatic potential obtained from DFT calculation. We will demonstrate that distortions observed in high-resolution STM/AFM experiments, including STM images of PTCDA, IETS images of CoPc [2,3] and bond order discrimination in C60 [4], are considerably affected by electrostatic force between local charge density in sample and atomic probe-particle (CO or Xe) attached to tip. [1] Hapala, P. et al., *Phys. Rev. B* **90**, 085421 (2014). [2] Chiang, C. et al., *Science* **344**, 885-8 (2014). [3] Hapala, P. et al., *Phys. Rev. Lett.* **113**, 226101 (2014). [4] Gross, L. et al., *Science* **337**, 1326-9 (2012).

O 15.9 Mon 17:00 MA 043

**Probing the Polar Nature of Bonds by means of Atomic Force Microscopy** — ●FLORIAN ALBRECHT<sup>1</sup>, MARTIN FLEISCHMANN<sup>2</sup>, MANFRED SCHEER<sup>2</sup>, MARTIN ONDRÁČEK<sup>3</sup>, PAVEL JELINEK<sup>3</sup>, and JASCHA REPP<sup>1</sup> — <sup>1</sup>Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — <sup>2</sup>Institute of Inorganic Chemistry, University of Regensburg, 93040 Regensburg, Germany — <sup>3</sup>Institute of Physics of Czech Academy of Science, 16253 Prague, Czech Republic

Recently, Kelvin probe force spectroscopy (KPF) has been shown to be a powerful tool to detect charge distributions with sub molecular resolution [1, 2]. We performed KPF measurements in a low temperature combined scanning tunneling and atomic force microscope with functionalized tips on different types of molecules - some of them exhibiting polar bonds. Whereas KPF represents the charge distribution with moderate resolution for large tip-molecule separations, it fails for short distances. We therefore introduce a novel technique, in which the dependence of the electric field on tip-sample distance is exploited to map out charges. Thereby, we were able to resolve the intramolecular charge distribution with unprecedented lateral resolution.

[1] F. Mohn, et al., *Nature Nano.* **7**, 227 (2012)

[2] B. Schuler, et al., *Nano Letters* **14**, 3342 (2014)

O 15.10 Mon 17:15 MA 043

**Response of a Kelvin probe force microscope to charge switching dynamics** — ●MARTIN ONDRACEK, PROKOP HAPALA, and PAVEL JELINEK — Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

Atomic or molecular structures which are capable of switching between two or more different charge states are of much interest as prospective building blocks for nanoelectronic devices. Kelvin probe force microscopy (KPFM), as a local and charge-sensitive probe, is a well-

sued tool for studying such structures. Indeed, charge switching has been already observed for Au atoms on NaCl using an atomic force microscope [L. Gross et al., *Science* **324**, 1428; J. Repp et al., *Science* **305**, 493]. However, the time scale of charging and discharging can vary over several orders of magnitude, depending on the particular structure, tip distance, voltage bias, substrate conductivity etc. When the charge dynamics is too fast to be probed in real time, it can still manifest itself as a deviation of the measured curves from perfect Kelvin parabolas and as a contribution to the the dissipation signal. We have developed a simple numerical simulator that models the charge dynamics and interaction of KPFM with the chargeable structure. This enables us to predict the dependence of the characteristic features showing up in KPFM measurements on the time scales of charging and discharging as well as on the instrumental time scales of KPFM: the oscillation period of the cantilever, response time of the feedback loop, and the acquisition time of one data point in the KPFM measurement.

O 15.11 Mon 17:30 MA 043

**Intermolecular Contrast in Atomic Force Microscopy Images without Intermolecular Bonds** — SAMPISA K. HÄMÄLÄINEN<sup>1</sup>, NADINE VAN DER HEIJDEN<sup>2</sup>, JOOST VAN DER LIT<sup>2</sup>, STEPHAN HARTOG<sup>2</sup>, PETER LILJEROTH<sup>2</sup>, and ●INGMAR SWART<sup>1</sup> — <sup>1</sup>Department of Applied Physics, Aalto University School of Science, Finland — <sup>2</sup>Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands

Atomic force microscopy (AFM) finds increasing use in the study of molecules on surfaces. This development started with the demonstration of imaging the chemical structure of organic molecules with atomic resolution.[1] Recently, features described to hydrogen bonds have also been reported. [2] These *intermolecular* bonds primarily have an electrostatic origin and may include some covalent character and other attractive interactions. However, it is not clear why these should yield significant repulsive contrast in AFM.

A recent theoretical study showed that the intermolecular features can be explained by the flexibility of molecule-terminated tips.[3] We probed this effect by carrying out atomic force microscopy experiments on a model system that contains regions where intermolecular bonds should and should not exist between close-by molecules. Intermolecular features are observed in both regions, demonstrating that intermolecular contrast cannot be directly interpreted as intermolecular bonds.[4]

[1] L. Gross et al. *Science*, **325**, 1110 (2009). [2] J. Zhang et al. *Science* **342**, 611 (2013). [3] P. Hapala et al., *Phys. Rev. B* **90**, 085421 (2014). [4] S.K. Hämäläinen et al., *Phys. Rev. Lett.* **113**, 186102 (2014).

O 15.12 Mon 17:45 MA 043

**Image Distortions of Molecules in Atomic Force Microscopy with Carbon Monoxide Terminated Tips** — ●NIKOLAJ MOLL, LEO GROSS, BRUNO SCHULER, ALESSANDRO CURIONI, 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) 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]. The underlying mechanisms of image distortions in AFM with CO-terminated tips are identified and studied in detail [2]. 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.

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

[2] N. 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).

O 15.13 Mon 18:00 MA 043

**Development of cryogen-free low temperature scanning probe microscope by using a closed cycle cryostat** — ●BYOUNG CHOI,

STEFAN ULRICH, and RYAN MURDICK — RHK Technology Inc. Troy, MI 48083, USA

Low temperature scanning tunneling microscope and atomic force microscope (LT-STM/AFM) based on a closed cycle cryostat (CCC) has been recently developed. We could realize to have the microscope thermally linked but mechanically decoupled to the cryostat by using a rubber bellows filled with Helium heat exchange gas. It enables atomically resolved topographic and spectroscopic measurements on various surfaces. At the temperature as low as 14K, the tip-sample distance fluctuation has been detected as low as 2 picometer after 8 hours of

cooling. With stable conditions of both microscope and controller, we could record more than 64 by 64 scanning tunneling spectra grid for over 10 hours. The lateral drift during the measurement was as low as 1 nanometer without a counter heater or a temperature controller. We will also present the high stability and reproducibility of the CCC-LT-STM/AFM with the atom resolved imaging of Si, Pt, Au and KBr surfaces with an STM and AFM combined imaging and spectroscopic technique. These results demonstrate that the CCC-LT-STM/AFM is an instrument enabling experiments on a variety of surfaces and materials at sub-angstrom resolution without using any liquid cryogen.