O 14: New Methods and Developments 2: Scanning Probe Techniques 2 (joint session O/KFM)

Time: Monday 15:00–16:15 Location: S053

O 14.1 Mon 15:00 S053

The importance of the dipole at the metal tip apex when approaching closer with a CO tip — •Shinjae Nam, Oliver Gretz, Thomas Holzmann, Alfred John Weymouth, and Franz J. Giessible — University of Regensburg, Regensburg, Germany

By functionalizing the tip with a single CO molecule, the resolution of atomic force microscope (AFM) can be drastically increased. The contrast enhancement produced by a CO tip has been explained in terms of strong Pauli repulsion and the associated tilting of the probe molecule. Although these two interactions play a dominant role at very close distances, recent experiments show that other interactions, especially electrostatic forces, are also important to understand the observed contrast. Here, we used Lateral Force Microscope, a variant of frequency modulation atomic force microscopy, to quantify the interaction between a CO tip and a CO on the Cu (111) surface. Interestingly, one more feature appeared in the measurement when we measured closer to the surface at the side of the surface CO. Following the results of other investigations, we include the electrostatic force in our simulations. We modeled our tip as a quadrupole, including a dipole at both the metal tip and on the CO molecules. We found that the dipole of the metal apex of the tip becomes a much greater influence as we approach closer to the surface.

O 14.2 Mon 15:15 S053

Chemical bond imaging using torsional and flexural higher eigenmodes of qPlus sensors — •Daniel Martin-Jimenez[1], Michael G. Ruppert[2], Alexander Ihle[1], Sebastian Ahles[3], Hermann A. Wegner[3], André Schirmeisen[1], and Daniel Ebeling[1] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen (Germany). — [2]University of Newcastle, Callaghan, NSW, 2308 (Australia). — [3]Institute of Organic Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen (Germany).

Non-contact atomic force microscopy (AFM) with CO-functionalized tips allows to visualize the chemical structure of adsorbed molecules and identify individual inter- and intramolecular bonds. Herein, we analyze the suitability of qPlus sensors, which are commonly used for bond imaging, for the application of modern multifrequency AFM techniques. Two different qPlus sensors were tested for submolecular resolution imaging via actuating torsional and flexural higher eigenmodes and via bimodal AFM. The torsional eigenmode of the first sensor is perfectly suited for performing lateral force microscopy (LFM) with single bond resolution. The advantage of using a torsional eigenmode is that the same molecule can be imaged either with a vertically or laterally oscillating tip without replacing the sensor simply by actuating a different eigenmode. Submolecular resolution is also achieved by actuating the 2nd flexural eigenmode of our second sensor. With laser Doppler vibrometry measurements and AFM simulations we can rationalize the image contrast mechanism of the 2nd eigenmode.

O 14.3 Mon 15:30 S053

3D Force mapping of single organic molecules at room temperature — •Timothy Brown, Philip Blowey, Jack Henry, and Adam Sweetman — University of Leeds, Leeds, UK

Scanning probe microscopy has established itself as a highly effective technique in the study of surfaces and molecules. In particular, non-contact atomic force microscopy has yielded enormous progress in our ability to characterise materials at the atomic scale, including the ability to resolve the chemical structure of individual molecules, and to acquire 3D force-maps with intramolecular resolution.

Intramolecular imaging is almost exclusively performed using qPlus sensors at cryogenic temperatures, as the functionalisation of the tip via a CO molecule (required for intra-molecular imaging) is only stable at near liquid helium temperatures. Although it has been shown that intramolecular imaging may be performed at higher temperatures, via use of semi-conducting, rather than metallic substrates, acquisition of high density 3D data sets generally requires long acquisition times. Hence the lack of thermal equilibrium between the tip and sample at room temperature makes acquisition of these datasets at elevated temperatures extremely challenging.

In this talk we present the first demonstration of high resolution 3D force mapping of a single organic molecule at room temperature using conventional silicon cantilevers. We show how the challenges of operating in a room temperature experimental environment can be overcome to acquire reproducible 3D force maps of a resolution and quality previously only demonstrated at low temperature.

O 14.4 Mon 15:45 S053

Monitoring of molecular configurations during manipulation with a scanning probe microscope — •Joshua Scheidt[1,2], Alexander Diener[1,2], Michael Maiworm[3], Rolf Findeisen[3], Kurt Driessens[2], F. Stefan Tautz[1], and Christian Wagner[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Jülich, Germany — [2]Maastricht University, Data Science and Knowledge Engineering, Maastricht, Netherlands — [3]Control and Cyber-Physical Systems Laboratory, Technische Universität Darmstadt, Darmstadt, Germany

A bold vision of nanofabrication is the assembly of functional molecular structures with a scanning probe microscope (SPM). Such an approach allows the quick variation of conformation and composition of (supra)molecular systems and an assessment of these parameters on the envisioned functionality. However, monitoring the molecular conformations during manipulations remain elusive due to the dual role of the SPM tip as an actuator and an imaging probe. We present an approach which enables monitoring based on continuously gathered force gradient data using a particle filter approach, which solves the inverse problem of conformation monitoring by comparing current force gradient data to a structured set of simulations stored in the form of a finite state automaton. This allows using molecular simulations with wall-times for completion much longer than the time scale of the experiments. Our proof-of-principle investigations are based on the vertical SPM manipulation of a PTCDA (3,4,9,10-perylene-tetracarboxylic dianhydride) molecule on the Au(111) surface.

O 14.5 Mon 16:00 S053

Real-space imaging of σ-hole by means of Kelvin probe force microscopy. — •Aurelio Gallardo[1], Benjamín Mallada[2], Bruno de la Torre[2], and Pavel Jelínek[1] — [1]FZU of the CAS, Prague, Czech Republic — [2]RCPTM-CATRIN, Palacký University, Olomouc Czech Republic

Anisotropic charge distributions on individual atoms, such as σ-holes, are crucial for the structural properties of certain systems. Nevertheless, the existence of σ-holes has only been demonstrated indirectly, either observing the interaction between halogenated molecules or by theoretical calculations. However, there was no experimental technique that would allow the spatail resolution of anisotropic atomic charges.

To tackle this problem, we employed Kelvin probe force microscopy (KPFM) which imaging mechanism relays on the electrostatic tip-sample interaction. To achieve the requested resolution, we developed a theoretical description of the KPFM imaging mechanism on atomic scale, which enables optimize the experimental setup. Namely we demonstrated both theoretically and experimentally that probe tip functionalization by a single Xe atom enhances the spatial resolution to directly visualize the anisotropic charge of the σ-hole, as well as the quadrupolar character of the carbon monoxide molecule. [1]

We believe that this work large already outstanding imaging capabilities of scanning probe techniques. In particular, this KPFM technique will enable better description of charge distribution in molecular complexes as well as on surfaces.

References: [1] Mallada et al., Science 374, 863-867 (2021)