O 68: Poster: Scanning Probe Techniques: Method Development

Time: Wednesday 18:00–20:00 Location: Poster C

O 68.1 Wed 18:00 Poster C

GXSM4 - an update — Percy Zahl[1] and •Thorsten Wagner[2] — [1]Center for Functional Nanomaterials, Brookhaven National Laboratory, USA — [2]Institute of Experimental Physics, Johannes Kepler University Linz, Austria

GXSM is an open-source software project with a history of more than 25 years[1−−3] and a worldwide user community[4] that provides a state-of-the-art control software for all types of scanning probe techniques (STM, AFM, ...). The fourth generation of this versatile tool is based on the latest GNOME/linux desktop and a digital signal processor (DSP). The build-in General Vector Probe (GVP) enables freely programmable spectroscopy (e.g. IV in case of STM, FZ in case of NC-AFM, ...) and manipulation/probing. Up to three arbitrary wave forms can directly control the coarse motion of the SPM (Besocke/Beetle, Koala, ...). The embedded Python interface can perform even more complex and automated tasks. Thus, it is only a small step to achieve AI-based image recognition and processing (via OpenCV) and automated scanning control.[5] We will summarize the recent achievments and give an outlook on future plans (e.g. RedPitaya/FPGA based hardware), but we are also happy to discuss issues and technical requirements from the community.

[1] P. Zahl et al. in Rev. Sci. Instrum. 74, 1222–1227 (2003)
[2] P. Zahl et al. in J. Vac. Sci. Technol. B28, C4E39 (2010)
[3] P. Zahl et al. in Imaging and Microscopy, 17, 38-41 (2015)
[4] gxsm.sf.net and github.com/pyzahl/Gxsm4
[5] Arias et. al. in J. Phys. Chem. A 127, 5959–6134 (2023)

O 68.2 Wed 18:00 Poster C

Enhancing AFM image analysis through machine learning with style translation and data augmentation — •Jie Huang[1], Niko Oinonen[1], Lauri Kurki[1], and Adam S. Foster[1,2] — [1]Department of Applied Physics, Aalto University, Helsinki, Finland — [2]WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma- machi, Kanazawa, Japan

Atomic Force Microscopy (AFM) is critical for atomic-scale nanostructure characterization. Simulations, especially using Particle Probe AFM (PPAFM), provide a cost-effective means for rapid image generation. Leveraging state-of-the-art machine learning models and substantial PPAFM-generated datasets, properties like molecular structures, electrostatic force potential, and molecular graphs can be accurately predicted using AFM images from simulations or experiments. However, transferring model performance from PPAFM to real AFM images poses challenges due to the subtle variations in real experimental data compared to the seemingly flawless nature of simulations. Our study explores Cycle GANs for style translation to augment data and improve the predictive accuracy of machine learning models in surface property analysis. Focused on mitigating the gap between simulated PPAFM and authentic AFM images, we optimize hyperparameters, showcasing the method's effectiveness through paired data comparisons. This research promises valuable insights, providing a novel approach to enhance machine learning model efficiency in the absence of abundant experimental data.

O 68.3 Wed 18:00 Poster C

On the origin and elimination of cross coupling between tunneling current and excitation in scanning probe experiments that utilize the qPlus sensor — Michael Schelchshorn, •Fabian Stilp, Marco Weiss, and Franz J. Giessibl — University of Regensburg, Institute of Experimental and Applied Physics, Universitätsstrasse 31, D-93040 Regensburg, Germany

The qPlus sensor allows for the simultaneous operation of scanning tunneling microscopy (STM) and atomic force microscopy (AFM). When operating a combined qPlus sensor STM/AFM at large tunneling currents, a hitherto unexplained tunneling current-induced cross coupling can occur, which has already been observed decades ago. Here, we study this phenomenon both theoretically and experimentally; its origin is voltage drops on the order of μV that lead to an excitation or a damping of the oscillation, depending on the sign of the current. Ideally, the voltage drops would be phase-shifted by $\pi/2$ with respect to a proper phase angle for driving and would, thus, not be a problem. However, intrinsic RC components in the current wiring lead to a phase shift that does enable drive or damping. Our theoretical model fully describes the experimental findings, and we also propose a way to prevent current-induced excitation or damping.

O 68.4 Wed 18:00 Poster C

Sample preparation for STM analysis — •Caroline Hommel, Lukas Spree, Luciano Colazzo, and Andreas Heinrich — Center for Quantum Nanoscience, 52 Ewhayeodae-gil, Daehyeon-dong, 03760 Seoul, South Korea

The process of sample preparation within ultra-high vacuum (UHV) settings crucially impacts the success of scanning tunneling microscopy (STM) experiments. While the sublimation of atoms and thermally stable, volatile molecules provides a pristine avenue to introduce analytes onto UHV surfaces, challenges arise when compounds lack volatility or thermal stability. In such instances, alternative methods become essential. Studies highlight solvent-based preparations like dropcasting as potentially beneficial, though they necessitate preparation outside the UHV chamber. An alternative, the electro spray deposition technique, proves effective by enabling molecules to traverse multiple pumping stages into UHV environments out of a solvent.

This technique's success hinges upon several critical parameters, including distance to the sample, solvent type, concentration, pressure, and duration. We investigate these parameters using functionalized fullerenes. Transitioning from bulk sample characterization of these intriguing compounds to investigating thin layers or individual molecules demands innovative methodologies to regulate interactions with the underlying substrate and effectively orientate the encapsulated species.

O 68.5 Wed 18:00 Poster C

Molecular behaviour during SPM tip functionalization for Scanning Quantum Dot Microscopy — •Paul Laubrock, Tim Dierker, and Philipp Rahe — Universität Osnabrück

Scanning quantum dot microscopy (SQDM) [1] is a variant of scanning probe microscopy (SPM) that enables the quantitative mapping of the electrostatic potential at the atomic scale [2]. A prerequisite for SQDM is the SPM tip functionalization with a (molecular) quantum dot. We developed an instructive flowchart for efficient preparation of functionalized SQDM tips based on scanning tunneling microscopy (STM) manipulation experiments at 5K with 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) molecules on Ag(111). Here we discuss experimental observations regarding the molecular behaviour in the tip-sample gap. In particular, we investigate an apparent instability in the STM signals appearing with a particular imaging contrast after lateral manipulation of a single PTCDA molecule. We interpret this and further observations in the context of dynamic bond formation/breaking in the surface-molecule-tip system.

[1] C. Wagner et al., PRL 115, 026101 (2015)
[2] C. Wagner et al., Nat. Mater. 18, 853 (2019)

O 68.6 Wed 18:00 Poster C

High-resolution characterization of single-step motion in piezoelectric friction-inertia walkers — •Felix Huber, Susanne Baumann, and Sebastian Loth — University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany

High precision positioners are a prerequisite for the realization and automation of cutting edge research experiments. Piezoelectric friction-inertia walkers offer the combination of high accuracy movement on the millimeter scale with a resolution on the nanometer scale and are essential for scanning probe microscopy (SPM) applications. The behavior and reliability of nanopositioners based on the friction-inertia principle strongly depends on the respective use of contact surface materials.

Here, we use optical interferometry to monitor the single step motion of a linear piezoelectric friction-inertia walker on the nanometer scale. We test different combinations of metallic and ceramic contact surface materials as well as contact surface geometries and identify material combinations that offer large step sizes or reliable single-step motion which can be implemented easily in home-built SPM setups.

O 68.7 Wed 18:00 Poster C

Automated tip preparation for electron spin resonance measurements in STM — •Lovis Hardeweg, Cathrin Haab, Wantong Huang, Paul Greule, Máté Stark, Christoph Sügers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

The development of scanning tunnelling microscopy (STM) combined with electron spin resonance (ESR) is a powerful technique to image and investigate spins on surfaces [S. Baumann et al. Science 350.6259 (2015), pp. 417-420]. However, it relies on spin-polarized tips and their preparation often requires time-consuming and repetitive work. Here, we present a multi-step routine based on supervised machine learning that autonomously creates ESR-active tips. It includes locating magnetic Fe atoms on MgO/Ag, MgO-layer thickness determination, tip evaluation/conditioning, as well as drift correction. Besides, the number of MgO monolayers on Ag is automatically determined and the individual Fe atoms are picked up onto the tip. Finally, the routine evaluates the ESR capabilities of the tip.

O 68.8 Wed 18:00 Poster C

Development and implementation of data model for scanning tunneling microscopy and scanning tunneling spectroscopy — •Yichen Jin[1], Rubel Mozumder[1], Yan Wang[2], Jürgen P. Rabe[1,3], Heiko B. Weber[4], Tamás Haraszti[5], Sabine Maier[4], Carlos-Andres Palma[2,3], Sandor Brockhauser[1], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin, Berlin, Germany — [2]Institute of Physics, Chinese Academy of Sciences, Beijing, PR China — [3]Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [4]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [5]Leibniz-Institut für Interaktive Materialien e.V., RWTH, Germany

Since the first realization of scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS), a wide range of applications has been developed by using the technique of quantum tunneling effect. The community aims at organize experimental data along FAIR principles, thereby developing or using a standard vocabulary of metadata. NeXus allows to generate such a sort of data modelling and with that we have developed specific data model called NX_sts for STM/STS experiment. Our work focuses not only on storing data and metadata from STM/STS experiments in terms of the NX_sts vocabulary but also supports handling data-analysis results. In this presentation, we will show how metadata can be converted into the NeXus data format. We will detail the basic software architecture of reader that transforms metadata file into STM/STS specific data model which in terns follows NeXus data format concepts.

O 68.9 Wed 18:00 Poster C

Towards light-wave scanning tunneling microscopy in strong magnetic fields — Victoria Ruckerbauer, •Felix Giselbrecht, Andreas Rank, Christoph Rohrer, Leo Ringer, Michael Betz, Christian Meineke, Jakob Schlosser, Rupert Huber, and Jascha Repp — Department of Physics, University of Regensburg, Regensburg, 93040, Germany

In light-wave-driven scanning tunneling microscopy (LW-STM) the tunneling junction is biased by an ultrashort laser pulse instead of having a static voltage [1]. This method enables combined Ångström and femtosecond spatiotemporal resolution as demonstrated by the direct observation of the ultrafast motion of a molecular orbital [2]. Combining this development with a tunable magnetic field would allow to follow spin dynamics – spin precession, for example – in molecules and other atomic structures with single-electron sensitivity. To this end, a novel LW-STM is being developed with an external magnetic field to resolve single-spin dynamics with atomic spatial and ultrafast temporal resolution. We will discuss the instrumental challenges of this development and present the resulting instrument design including the STM head, the laser source as well as the solution to introduce the laser transient from outside the vacuum system to the STM junction. [1] Cocker *et al.*, Nature Photonics **7**, 620 (2013), [2] Cocker *et al.*, Nature **539**, 263 (2016).

O 68.10 Wed 18:00 Poster C

Non-contact AFM experiments with a diamond tip equipped needle sensor: From field emission to tunneling — •Stefan Schulte[1,2], Sven Just[1,3], Victor I. Kleshch[4], F. Stefan Tautz[1,3], and Ruslan Temirov[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Cologne, Germany — [3]Fundamentals of Future Information Technology, Jülich Aachen Research Alliance (JARA), Jülich, Germany — [4]Moscow, Russia

A length extension quartz resonator (needle sensor) equipped with a CVD-grown single crystal diamond needle on the tip is characterized in a room-temperature AFM setup at UHV conditions. The particular setup allows for simultaneous AFM, field emission and tunneling experiments. The diamond tip needle sensor could be a platform to enable the measurements of electrostatic surface potential in scanning quantum dot microscopy (Wagner et al., Phys. Rev. Lett., 2015). We focus on the transition from a non-conductive state of the diamond to a surface-conductive state, which occurs when the surface of the diamond needle is transformed into amorphous carbon at elevated field emission currents. The current-voltages characteristics of the diamond needle are recorded at different distances ranging from the attractive AFM regime to several nm above the surface. Simultaneously recorded AFM signals of the resonant behavior of the sensor reveal the specific transformation processes. Finally, the conductive diamond tip enables tunneling experiments at comparably low bias voltages.

O 68.11 Wed 18:00 Poster C

Development of a Fast In Situ Scanning Tunneling Microscope for Studies of Electrochemical Interfaces — •Knud Schröter, Fabian Schröfel, Matthias Greve, Karsten Tarhouni, and Olaf Magnussen — Institut für Experimentelle und Angewandte Physik, Kiel

The atomic-scale understanding of processes at the interface between solid electrodes and liquid electrolytes is of high importance for electrochemical energy storage and conversion. Electrochemical scanning tunneling microscopy (ECSTM) is a key technique for the investigation of these interfaces and as such, it has seen widespread use. However, image acquisition in conventional ECSTM is a rather slow process, requiring tens of seconds or minutes per image. To help understand the precise reaction mechanisms of atomic and molecular species at solid-liquid interfaces, their movement and interactions need to be resolved.

For this, high-speed STMs capable of operating at rates >10 images per second are necessary. However, this technique has not been widely employed, mainly because of the instrumental requirements.

In this contribution, we present a new high-speed ECSTM developed and built in our group based on a Nanonis SPM controller. The instrument includes a novel scanner design with two independent piezo stacks for slow wide-range motion and local high-speed motion and a custom high-bandwidth preamplifier integrated into the scan head as close as possible to the tip. We will show first results on the implementation of the fast imaging mode.

O 68.12 Wed 18:00 Poster C

Automated STM imaging and spectroscopy: porphyrin molecular arrays as an exemplar — •Matthew Edmondson and Alex Saywell — School of Physics & Astronomy, University of Nottingham, UK

Materials analysis via scanning probe microscopy (SPM) is often labour intensive and not standardised to the level of the procedures employed within characterisation techniques such as nuclear magnetic resonance (NMR) and mass spectrometry. While SPM approaches provide impressive atomic/sub-molecular spatial resolution, [1] and allow characterisation of electronic states, a key challenge is to obtain statistically sufficient measurements over the panoply of features present on the material under study. Molecular overlayers, specifically the often-studied porphyrin-based assemblies on metals [2], provide a test-platform for the automated spatial and electronic characterisation of a molecule-substrate system. Porphyrin molecules may undergo various on-surface process (e.g. ring-closing, metalorganic coordination, and self-metalation) with a resultant change in electronic states potentially offering a ‘fingerprint’ of the chemical and structural changes.

Here, we present details of a semi-automated approach to characterising a molecule-substrate system. Custom SPM imaging and spectroscopy routines have been developed to interface with commercial control electronics and provide a route towards automated data collection.

[1] A. Sweetman, N.R. Champness, A. Saywell, Chem. Soc. Rev., 2020, 49, 4189 [2] Gottfried, J. M., Surf. Sci. Rep., 2015, 70, 259